ENVIRONMENTAL PROTECTION

Esa Nikunen • Riitta Leinonen
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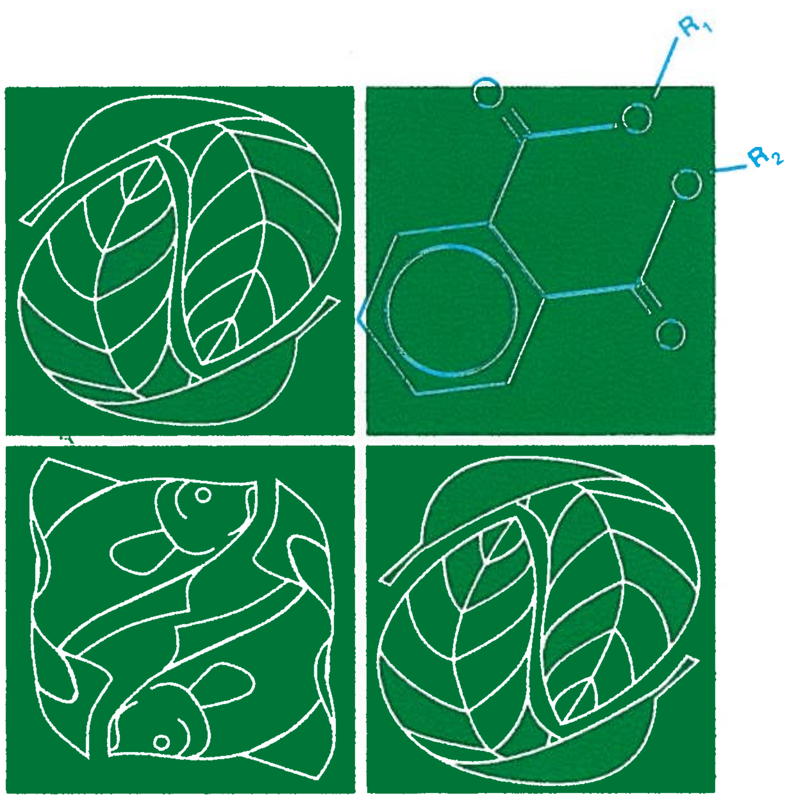
Environmental properties of chemicals

Volume 1



FINNISH ENVIRONMENT INSTITUTE • EDITA

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Preface

The assessment of the environmental impact of chemical substances is a complex issue. In order to be able to even roughly evaluate the environmental fate and effects a great deal of basic data are needed. Often one of the most difficult tasks in this respect is locating results of past testing which would be necessary in completing the above mentioned evaluation. In many cases even the most basic data on the inherent properties of different chemical substances are lacking.

The first handbook on the Environmental Properties of Chemicals was published by the Finnish Ministry of the Environment (report 91/1990) in 1990. This handbook represents its second revised version. There are now approximately 300 new substances dealt with and more information has been collected on many of the substances present in the first edition as well.

This handbook has been compiled from the Data Bank of Environmental Properties of Chemicals collected by the Finnish Environment Institute (earlier the National Board of Waters and the Environment). The aim of this register has been to, for example, facilitate the environmental impact assessment and the environmental classification of chemical substances. This basic ecotoxicological data on chemicals can , of course, be used for many different purposes.

The information is mainly derived from scientific literature, handbooks and other material at the disposal of Finnish environmental authorities. This compilation of basic information started in 1985 when the Finnish Ministry of the Environment ordered a series of reports concerning the hazards of different substances. One of the reports dealt with the toxicity of chemicals to aquatic organisms (Nikunen et al. 1986) and this collection of data on the effects of about 1000 substances was compiled into a register. Since then this register has been improved and new data has been collected systematically. Today, the register is also available as an online version as well as a PC version.

The quality of the data in the register in terms of, for example, the way in which tests have been conducted has not in all cases been verified. Consequently, neither the authors nor the Finnish Environment Institute take responsibility for the possible faults in this book.

The authors wish to acknowledge the help that has been given, e.g. by Ms. Eeva Hottinen, Mr. Hannu Hukkanen, Ms. Kirsti Karkinen, Ms. Marja-Liisa Lindell and Mr. Joel Pottala.

Contents

1 Contents of the report

1.1 General

The database contains information on 2,073 substances. The substances are either chemical sub stances or commercial products. The data on each chemical forms a document. Consequently the database consists of 2,073 documents. The documents are numbered and listed in alphabetical order. These running numbers are used for listing the chemicals. Since there are a lot of synonymous names to chemicals, Index I contains all the chemical names and synonyms in alphabetical order. In Index II chemicals are listed by their CAS numbers (Chemical Abstract Service Registry number). Chapter 4 contains the documents with the information on environmental properties. The abbreviations, definitions and explanations are available in Chapter 2. Chapter 3 contains the scientific, English and Finnish names of exposed species mentioned in database. The references are listed in Chapter 5.

1.2 The collection of data

The report data was mainly compiled from scientific publications, handbooks and databases in the field of ecotoxicology which have been available to environmental protection authorities. The scientific value of the compiled information has not been assessed. The authors are not responsible for possible mistakes in the publication.

1.3 Structure of the document

Each document of a chemical consists of six sections. Underneath the section name the possible headings are listed. The amount of data and consequently the number of headings used varies considerably depending on the chemical in question.

The heading of the document consists of the chemical number which is a running number, chemical name (commercial products are marked with *) and CAS number (Chemical Abstract Service Registry number).

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Dissociation constant of base K_b or pK_b
Dissociation percentage
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Log air/water coefficient, log P_{aw}
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LDLo values to mammals in non-oral exposure, mg/kg
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LCLo values to mammals in inhalation exposure, ppm
TDLo values to mammals in oral exposure, mg/kg
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LCLo values to birds in inhalation exposure, mg/m^3
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EC50 values to algae, mg/l
LOEC values to algae, mg/l
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EC50 values to crustaceans, mg/l
LOEC values to crustaceans, mg/l
NOEC values to crustaceans, mg/l
LC50 values to fishes, mg/l
EC50 values to fishes, mg/l
LOEC values to fishes, mg/l
NOEC values to fishes, mg/l
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Effects on the reproduction of aquatic organisms
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Other effects on aquatic ecosystems
Other information

1.4 Locating the chemicals

The chemicals are listed in alphabetical order. In order to facilitate the process of locating chemicals for example by synonymous name or CAS-number, there are two indexes at the end of the report. Index I, is an Alphabetical List of Chemicals and Index II, is a List of Chemical Abstract Service Registry Numbers.

Index I is an alphabetical listing of the chemicals according to both their most common name and other synonymous names. The number next to the chemical's name refers to the document number.

The CAS numbers (American Chemical Society's Chemical Abstract Service Registry Number) are to be found in Index II. CAS numbers are used worldwide in scientific literature and they permit absolute identification of a chemical.

1.5 Interpretation of test results

There are many different ways to express test results in words. No one of them is necessarily scientifically any better than any other. The following classification has been used by the Chemicals Division of the Finnish Environment Institute for various purposes. They offer guidance especially to those who are not familiar with the interpretation of the numerical values of test results.

Toxicity

Acute toxicity to earthworms

Test in soil LC_{50} (mg/kg dry soil)	Class
< 1	highly toxic
1–10	toxic
10–100	moderately toxic
100–1000	slightly toxic
> 1000	very slightly toxic

Acute and subacute toxicity to birds

Acute oral LD_{50} (mg/kg body weight)	Feeding study LC_{50} (mg/kg food)	Class
< 10	< 50	highly toxic
10–50	50–500	toxic
50–500	500–1000	moderately toxic
500–2000	1000–5000	slightly toxic
> 2000	> 5000	very slightly toxic

Acute toxicity to bees

LD_{50} oral µg/bee	Class
< 0.1	highly toxic
0.1–1.0	toxic
1–10	moderately toxic
10–100	slightly toxic
> 100	very slightly toxic

Acute toxicity to aquatic organisms

LC/EC/IC50 mg/l	Class
< 1	highly toxic/very toxic
1–10	toxic
10–100	slightly toxic/harmful
> 100	very slightly toxic

Chronic toxicity to aquatic organisms

NOEC mg/l	Class
< 0.01	highly toxic/very toxic
0.01–0.1	toxic
0.1–1.0	slightly toxic/harmful
> 1.0	very slightly toxic

Acute toxicity to mammals

Acute oral LD_{50} mg/kg body weight	Acute dermal LD_{50} mg/kg bw	Acute inhalation LC_{50} mg/l in air/4 h	Class
< 25	< 50	< 0.5	very toxic
25–200	50–400	0.5–2	toxic
200–2000	400–2000	2–20	harmful
> 2000	> 2000	> 20	very slightly toxic

Degradation

Readily biodegradable substances:

If in the OECD 28-day ready biodegradability studies the following levels of degradation are achieved:

– in tests based upon dissolved organic carbon: 70 %
– in tests based upon oxygen depletion or carbon dioxide generation: 60 % of the theoretical maxima.

These levels of biodegradation must be achieved within 10 days of the start of degradation, which point is taken as the time when 10 % of the substance has degraded.

Biodegradability can also be evaluated using the ratio of BOD5/COD. If the ratio is 0.5–1.0 the substance can be considered readily biodegradable.

Inherently biodegradable substances:
A substance which in an OECD Inherent biodegradability test achieves the following levels:

- more than 20 % biodegradation, may be regarded as evidence for inherent primary biodegradability
- more than 70 % mineralisation, may be regarded as evidence for ultimate biodegradation.

Degradation in soil

Half-life, $t_{1/2}$	Class
< 1 week	readily degradable
1 week–1 month	fairly readily degradable
1–3 months	fairly slightly degradable
3–8 months	slowly degradable
> 8 months	very slowly degradable

Mobility

Volatility

Vapour pressure P_{vp} (Pa), (20–25 °C)	Class
> 100	highly volatile
1–100	volatile
0.01–1	moderately volatile
0.0001–0.01	slightly volatile
< 0.0001	very slightly volatile

Volatility from water

Henry's law constant (H) H (atm m³/mol)	H (Pa m³/mol)	Class
$> 10^{-3}$	> 100	highly volatile
10^{-5}–10^{-3}	1–100	volatile
10^{-7}–10^{-5}	10^{-2}–1	slightly volatile
$< 10^{-7}$	$< 10^{-2}$	very slightly volatile

Water solubility

S (mg/l)	Class
> 1000	readily soluble
10–1000	moderately soluble
0.1–10	slightly soluble
< 0.1	very slightly soluble

Mobility in soil

K_{oc}	K_d	Class
< 50	< 0.75	very highly mobile
50–150	0.75–2.25	highly mobile
150–500	2.25–7.5	moderately mobile
500–2000	7.5–30	slightly mobile
2000–5000	30–75	very slightly mobile
> 5000	> 75	immobile

Bioaccumulation

BCF	log Kow	Class
< 100	< 3	slightly accumulating
100–1000	3–5	moderately accumulating
> 1000	5	highly accumulating

2 Environmental properties of chemicals

Guide to the Handbook Entries

chemical number — chemical name — synonymous names of chemical or commercial (*) products — CAS-number

1 • Abate 3383-96-8

Synonyms	0,0-Dimethylphosphorothioate-0,0-diester with 4,4'-thiodiphenol 0,0,0',0'-Tetramethyl-0,0-thiodi-p-phenylene phosphorothioate Abathion Temephos	
Use	Mosquito larvicide.	
Molecular weight	466.48	
LD50 values to mammals in oral exposure mg/kg	8600 orl-rat, act (Pesticide Dictionary 1976) 1000 orl-rat (Lewis & Sweet 1984)	reference; see list in Vol. 2 Ch. 5
LD50 values to mammals in non-oral exposure, mg/kg	> 400 skn-rbt (Verschueren 1983) 1370 skn-rat (Lewis & Sweet 1984) 970 skn-rbt	exposed species; see list in Vol. 2 Ch. 3.2
LD50 values to birds in oral exposure, mg/kg	32 orl-bwd 50 orl-pgn 79 orl-dck (Lewis & Sweet 1984) 42.2 orl-Agelaius phoeniceus > 100 orl-Sturnus vulgaris 75 orl-Coturnix coturnix 31.6 orl-Passer domesticus 56.2 orl-Carbodacus mexicanus (Schafer et al. 1983)	exposed species; see list in Vol. 2 Ch. 4
Effects on arthropods	100% mortality or 0% survival including algicidal anherbicidal effects: Culex sp., 25 g/ha, 2 days; LC50 0.000731 mg/l, 1 day, Culex pipiens; LC50 0.001165 mg/l, 1 day, Culex pipiens (Helson & Surgeoner 1986). 100% mortality or 0% survival including algicidal and herbicidal effects: Aades sp. 0.030 mg/l, 1 day (Fortin et al. 1987).	
LOEC values to algae, mg/l	0.1 pht, act, Dunaliella euchlora Phaeodactylum tricornutum Skeletonema costatum (Verschueren 1983)	abbreviations; see list in Vol. 2 Ch. 3
LC50 values to crustaceans, mg/l	0.082 96 hr, Gammarus lacustris (Sanders 1969) 0.045 72 hr Metapenaeus monoceros Penaeus monodon (Tsai 1978)	exposure time; see list in Vol. 2 Ch. 3.4

1 • Abate

3383-96-8

Synonyms	0,0-Dimethylphosphorothioate-0,0-diester with 4,4'-thiodiphenol 0,0,0',0'-Tetramethyl-0,0-thiodi-p-phenylene phosphorothioate Abathion Temephos	
Use	Mosquito larvicide.	
Molecular weight	466.48	
LD50 values to mammals in oral exposure mg/kg	8600 1000	orl-rat, act (Pesticide Dictionary 1976) orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	> 400 1370 970	skn-rbt (Verschueren 1983) skn-rat (Lewis & Sweet 1984) skn-rbt
LD50 values to birds in oral exposure, mg/kg	32 50 79 42.2 > 100 75 31.6 56.2	orl-bwd orl-pgn orl-dck (Lewis & Sweet 1984) orl-Agelaius phoeniceus orl-Sturnus vulgaris orl-Coturnix coturnix orl-Passer domesticus orl-Carbodacus mexicanus (Schafer et al. 1983)
Effects on arthropods	100% mortality or 0% survival including algicidal anherbicidal effects: Culex sp., 25 g/ha, 2 days; LC50 0.000731 mg/l, 1 day, Culex pipiens; LC50 0.001165 mg/l, 1 day, Culex pipiens (Helson & Surgeoner 1986). 100% mortality or 0% survival including algicidal and herbicidal effects: Aades sp. 0.030 mg/l, 1 day (Fortin et al. 1987).	
LOEC values to algae, mg/l	0.1	pht, act, Dunaliella euchlora Phaeodactylum tricornutum Skeletonema costatum (Verschueren 1983)
LC50 values to crustaceans, mg/l	0.082 0.045	96 hr, Gammarus lacustris (Sanders 1969) 72 hr Metapenaeus monoceros Penaeus monodon (Tsai 1978)
EC50 values to crustaceans, mg/l	0.0136 0.0004	0.21 d, Cyclopoida 0.5 d, Daphnia sp. (Helgen et al. 1988)
LC50 values to fishes, mg/l	0.158 0.023 7.5 0.6 1.24 11.4 1.9 0.47 0.16	96 hr, Salmo gairdneri (FPRL 1971) 72 hr, Mugil sp. 72 hr, Anguilla anguilla 72 hr, Mugil cephalus (Tsai 1978) 48 hr, Aplocheilus lineatus 48 hr, Macropodus cupatus (Jacob et al.1982) 96 hr, Poecilia reticulata 96 hr, Sarotheredon galilaea (Kpekata 1983) 96 hr, Salmo gairdneri (Verschueren 1983)

A

Effects on the reproduction of water organisms	Laccotrophes griseus, 10 d, 0.050 mg/l, reproductive effect (Mathavan & Jayakumar 1987).
Other information of water organisms	Dunaliella euchlora: 1000 ppb (36% reduction in 02 evolution) Dunaliella euchlora: 100 ppb (23% reduction in 02 evolution) Phaeodactylum tricornutum: 100–0 ppb (38% reduction in 02 evol.) Phaeodactylum tricornutum: 100 ppb (28% reduction in 02 evol.) Skeletonema costatum: 1000 ppb (55% reduction in 02 evolution) Skeletonema costatum: 100 ppb (23% reduction in 02 evolution) Cyclotella nana: 1000 ppb (80% reduction in 02 evolution) (Earnest 1976) Aedes caspius, LC50 0.0013 mg/l; Aedes excrucians, LC50 0.0012 mg/l; Aedes punctor, LC50 0.0021 mg/l; Aedes quasirusticus, LC50 0.0016 mg/l; Aedes rusticus, LC50 0.0029 mg/l; Aedes vexans, LC50 0.0020 mg/l; Anopheles atroparvus, LC50 0.0047–0.0138 mg/l; Culex pipiens, LC50 0.001 mg/l; Culex theileri, LC50 0.0019–0.0058 mg/l; (Grandes & Sagrado 1988). Invertebrates, 0.33 d, 0.0009–0.0042 mg/l, change in number of species groups in a community; Diaptomus sp., 0.83 d, 0.006 mg/l, mortality; Chaoborus sp. EC50, 1 d, 0.0012 mg/l; Ceriodaphnia sp., 0.0052 mg/l, 1 d, lethal effect (Helgen et al. 1988). Dugesia tigrina, 3 d, 10 mg/l, mortality; Dugesia dorotocephala, 3 d, 10 mg/l, mortality (Nelson et al. 1988).

2 • Abietic acid

514-10-3

Synonyms	Sylvic acid Abietinic acid	
Sumformula of the chemical	C19H29COOH * phenanthrene ring system	
Use	Major active ingredient of rosin.	
State and appearance	Yellowish resinous powder.	
Molecular weight	302.44	
Melting point	172–175	
LC50 values to crustaceans, mg/l	6.2	96 hr, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l°C	0.56	96 hr, Oncorhynchus kisutch (Leach & Thakore 1975)
	0.7	96 hr, Salmo gairdneri (Leach & Thakore 1976)
	0.41	96 hr, Oncorhynchus kisutch (Anon.1981)

3 • AC 222 *

70124-77-5

Synonyms	AC 705 Flusythrinate
Active ingredients	((+-)cyano(3-fenoxyphenyl)methyl(+-)-4-difluoromethoxy)-alfa-; (1-methylethyl)benzeneacetate * 80.6%
Use	Insecticide (synthetic pyretroid).

LOEC values to fishes, mg/l	0.00007 srv, act, Pimephales promelas (Spehar et al. 1983)
NOEC values to fishes, mg/l	0.00003 srv, act, Pimephales promelas (Spehar et al. 1983)

4 • Acenaphthene

83-32-9

Synonyms	1,8-Hydroacenaphthylene Ethylenenaphthalene Periethylenenaphthalene 1,8-Ethylenenaphthalene
Sumformula of the chemical	C12H10
Purity, %	98 technical grade
Use	Manufacturing source: petroleum refining; shale oil processing; coal tar distilling. Users and formulation: dye and plastic manufacturing; insecticide and fungicide manufacturing. Natural sources (water and air): coal tar. Man caused sources (water and air): combustion of tobacco; constituent in asphalt; in soots generated by the combustion of aromatic fuels doped with pyridine (EPA 1975, Krishnan et al. 1979)).
State and appearance	White crystalline solid at room temperature, insoluble, denser than water. Will sink.
Odour	Threshold odour concentration in water at room temperature: 0.08 ppm, range 0.02–0.22 ppm, 14 judges. 20% of population still able to detect odour at 0.026 ppm 10% 0.014 1% 0.0019 0.1% 0.00021 (Lillard et al. 1975).
Molecular weight	154.21
Specific gravity (water=1)	1.189 1.069 technical grade
Vapour density (air=1)	5.32
Vapour pressure, mmHg	0.001–0.01
Water solubility, mg/l	0.57 (MITI 1992)
Melting point, °C	93–95 (MITI 1992)
Boiling point, °C	277.2 (MITI 1992)
Log octanol/water coefficient, log Pow	4.33 (Sax 1986) 3.92 (Chin et al. 1986) 3.92 (Mackay 1982) 3.92 (Sangster 1989) 4.18 (MITI 1992)
Adsorption/desorption	Aquatic reactions: adsorption on smectite clay particles from simulated seawater at 25% -experimental conditions: 100 µg acenaphthene /l, 50 mg smectite /l: adsorption: nil (Meyers & Oas 1978).
Photochemical degradation in soil	Acenaphthene resists photochemical degradation in soil (Sax 1986).

A

Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	387 489–1000 254–1270	bluegill (Sax 1986) 8w, Cyprinus carpio, conc 0.03 mg/l 8w, Cyprinus carpio, conc 0.003 mg/l (MITI 1992)
LD50 values to mammals in oral exposure, mg/kg	10000 2100	orl-rat, act orl-mus, act (Sax 1986)
Effects on the physiology of mammals	Orl in olive oil, 2000 mg/kg, 32 d, daily, young rat: body weight loss, enzyme and blood changes, mild liver and kidney damage, mild bronchitis (Sax 1986). Inhalation, rat, 4 hr/d, 6d/w, 12 mg/m³: toxic effect on blood, lungs, and glandular constituents (Sax 1986).	
Health effects	Irritating to skin and mucous membranes. May cause vomiting if large amounts are ingested (Sax 1986).	
Mutagenicity	Mutagenicity: acenaphthene induced significant mutation to 8-azaguanine resistance in Salmonella typhimurium at concentrations as low as 1000 μM (Verschueren 1983).	
Effects on wastewater treatment	Since polychlorinated PAH are probably high toxic to aquatic organisms and persistent in the environment as are polychlorinated biphenyls and polychlorinated naphthalenes, chlorination for purification of wastewaters or drinking waters containing high concentrations of PAH's may be inadvisable. Activated sludge treatment is unable to oxidize PAH's within normal retention times (Sax 1986).	
LC50 values to crustaceans, mg/l	41	48 hr, Daphnia magna (LeBlanc 1980)
EC50 values to crustaceans, mg/l	41.2	48 hr, Daphnia magna (Sax 1986)
LC50 values to fishes, mg/l	1.6 1.72 0.67 0.58 1.7 > 400	96 hr, flow-through, Pimephales promelas 96 hr, flow-through, Ictalurus punctatus 96 hr, flow-through, Salmo gairdneri 96 hr, flow-through, Salmo trutta m. lacustris (Holcombe et al. 1983) 96 hr, Lepomis macrochirus (Buccafusco et al. 1981) 48 hr, Oryzias latipes (MITI 1992)
LOEC values to fishes, mg/l	0.97 0.56	srv, schr, Cyprinodon variegatus (Ward & Parrish 1980) srv, grw, schr, Pimephales promelas (Cairns & Nebeker 1982)
NOEC values to fishes, mg/l	0.34	srv, grw, schr, Pimephales promelas (Cairns & Nebeker 1982)
Other information about water organisms	In most cases, crustaceans are the most sensitive aquatic organisms to polycyclic aromatic hydrocarbons. Fish are he most resistant. Polychaete worms show intermediate sensitivity. Acenaphthene is only slightly toxic or practically non-toxic to mammals (Sax 1986). LC50, > 2.040 mg/l, 96 hr, flow-through, Aplexa hypnorum (Holcombe et al. 1983).	

Other effects on aquatic ecosystems	Oxidation of any polycyclic aromatic hydrocarbon (PAH) by chlorine and ozone, when used for the disinfection of drinking water, forms quinones. Chlorinating agents will also produce chlorine-substituted PAH's as well as oxidation products. The half-life for the reaction of all PAH's with chlorine is less than 0.5 hour. Hydrolysis is not significant. Photo lysis in an aquatic environment may be an important fate process, especially for the dissolved portion. Evaporation of lower-molecular-weight PAH's may be significant only in a clear, rapidly flowing shallow stream. Movement via sediment is considered to be an important transport process for PAH's. An exchange equilibrium exists in natural water systems between absorbed and soluble PAH's. Although the particulate form isfavored, a significant fraction of the PAH will be dissolvedexcept in systems that are very heavily contaminated by PAH's.PAH's with fewer than four rings are degraded by microbes andare readily metabolized by multicellular organisms.Biodegradation is considered to be the ultimate fate process.However, the concentration of bacteria and fungi capable ofoxidizing hydrocarbons are extremely low in all but heavilypolluted fresh and marine waters. Most species cannot use PAH's as a sole carbon source. Microbial oxidation of PAH's requiresoxygen and will not proceed in anoxic sediments or water (Sax 1986).

5 • Acenaphthylene

208-96-8

Use	Manmade sources: in soots generated by the combustion of aromatic hydrocarbon fuels doped with pyridine (Krishnan 1979).
Molecular weight	152.2
Specific gravity (water=1)	0.899
Water solubility, mg/l	3.93 at 25 °C in distilled water < 100 (MITI 1992)
Melting point, °C	80–83 89–91 (MITI 1992)
Boiling point, °C	280
Log octanol/water coefficient, log Pow	4.07 observed (Chin et al. 1986) 3.93 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	237–505 8w, Cyprinus carpio, conc 0.05 mg/l 225–545 8w, Cyprinus carpio, conc 0.005 mg/l (MITI 1992)
Mutagenicity	Did not induce significant mutation to 8-azaguanine resistance in Salmonella typhimurium at concentrations up to 1300 uM, the limit of solubility under the assay condition (Verschueren 1983).
LC50 values to fishes, mg/l	185 48 hr, Oryzias latipes (MITI 1992)

6 • Acephate

30560-19-1

Synonyms	Acetylphosphoramidothioic acid 0,S-dimethyl ester 0,S-Dimethylacetylphosphoroamidothioate Orthene
Sumformula of the chemical	C4H10NO3PS

Products containing the chemical	Ortho 12420 Orthene	
Molecular weight	183.18	
LD50 values to mammals in oral exposure, mg/kg	321 233 700	orl-mam orl-mus orl-rat (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	700 351 380 321 2000	unk-rat unk-mus unk-Peromyscus leucopus unk-Microtus pennsylvanicus (Virtanen & Nuuja 1987) skn-rbt (Sweet 1987)
LDLo values to mammals in oral exposure, mg/kg	681	orl-dog (Sweet 1987)
LCLo values to mammals in inhalation exposure, mg/kg	2200	5 hr, ihl-mus (Sweet 1987)
Mutagenicity	Unscheduled DNA synthesis: human: fibroblast, 1000 mg/l; gene conversion and mitotic recombination: S. cerevisiae; 50000 ppm; gene mutation in mammalian cells: mouse, lymphocyte, 1000 mg/l; microbial mutation without S9: E.coli, 5 mg/plate; S. typhimurium, 3 mg/plate; microsomal assay: S. typhimurium, 50 mg/plate; S. cerevisiae, 3 pph; sister chromatid exchange: hamster, ovary, 2000 mg/l (Sweet 1987).	
LD50 values to birds in oral exposure, mg/kg	106 852 350	orl-domestic bird orl-chicken orl-dck (Sweet 1987)
Effects on plants	Increases in either fertilizer level or temperature resulted in increased levels of phytotoxicity when plants were sprayed with recommended rates (0.4 g/l) of acephate (Chase & Poole 1984).	
LC50 values to crustaceans, mg/l	3.8 7.3	act, Penaeus duorarum 96 hr, Mysidopsis bahia (Anon. 1981, EPA 600/4-81-041)
LC50 values to fishes, mg/l	2740 1880 85	96 hr, Salmo gairdneri (Geen et al. 1984) 24 hr, Salmo gairdneri (Duangsawasdi & Klaverkamp 1979) 96 hr, Lagodon rhomboides (Anon. 1981)
EC50 values to fishes, mg/l	12600	phy, act, Salmo gairdneri (Watson et al. 1984)
Effects on the physiology of water organisms	Salmo gairdneri, 1 d, 100–400 mg/l, enzyme effect (Zinkl et al. 1987).	

7 • Acetaldehyde

75-07-0

Synonyms	Ethanal Ethylaldehyde Acetic aldehyde

Sumformula of the chemical	CH3CHO
Use	Manufacturing source: organic chemical manufacturing. Users and formulation: organic chemical manufacturing; perfumes, flavours, aniline dyes, plastics, synthetic rubbers manufacturing, silvering mirrors, hardening gelatin fibres. Natural sources (water and air): metabolic intermediate in higher plants; alcohol fermentation; sugar decomposition in body; by-product of most hydrocarbon oxidations. Man caused sources (water and air): vehicle exhaust; open burning and incineration of gas, fuel oil and coal; evaporation of perfumes; lab use (EPA 1975).
State and appearance	Colourless liquid or gas.
Odour	Characteristic. Quality: green sweet, apple ripener (Leonardos 1969) Hedonic tone: pungent (Verschueren 1983) Odour index: 5000000 (Verschueren 1983)
Molecular weight	44.1
Specific gravity (water=1)	0.783 at 18/4 °C
Conversion factor, 1 ppm in air=	1.831
Conversion factor, 1 mg/m³ in air=	0.55
Vapour pressure, mmHg	740 20 °C
Water solubility, mg/l	15488 (Leahy 1986)
Melting point, °C	-121 (Suntio et al. 1988) -123.5 (MITI 1992)
Boiling point, °C	20.2 21 (MITI 1992)
Log octanol/water coefficient, log Pow	0.42 (calc.) -0.47 (Leahy 1986) 0.45 (Sangster 1989)
Henry's law constant, Pa x m³/mol	290.7 calc. (Suntio et al. 1988) 10.18 calc. (Yaws et al. 1991)
Total degradation in water	Biodegradation: 80% by BOD period: 14d substance: 100 mg/l sludge 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	1930 single dose, orl-rat (Verschueren 1983)
LD50 values to mammals in non-oral exposure, mg/kg	640 scu-rat (Verschueren 1983)
LC50 values to mammals in inhalation exposure, ppm	20500 ihl-rat, 30 min (Verschueren 1983)
Health effects	Man: eye irritation sensitive persons: 25 ppm,15 min. eye irritation:50 ppm,15 min. irritation of respiratory tract: 134 ppm,30 min. irritation of nose and throat:200 ppm,15 min.

LC50 values to crustaceans, mg/l	3715–6772 2 days, Ceriodaphnia dubia 9268–14221 2 days, Daphnia magna (Takahashi et al. 1987)
LC50 values to fishes, mg/l	53 96 hr, Lepomis humilis (McKee & Wolf 1963) 53 96 hr, Lepomis macrochirus (Kemp et al. 1973)
Other information about water organisms	Anabaena cylindrica: 0.97%, EC50, growth, 10 days Anabaena inaequalis: 1.02%, EC50, growth, 10 days Anabaena sp.: 0.80%, EC50, growth, 10 days Anabaena variabilis: 1.27%, EC50, growth, 10 days Nostoc sp.: 2.87%, EC50, growth, 10 days (Stratton 1987).

8 • Acetamide

60-35-5

Synonyms	Ethanamide Acetic acid amine
Sumformula of the chemical	CH3CONH2
Use	Organic synthesis; general solvent; lacquers; explosives; wetting agent
Odour	Odour threshold: recognition: 140–160 mg/m³
Molecular weight	59.07
Specific gravity (water=1)	1.159 at 20/4 °C
Water solubility, mg/l	975000 20 °C
Melting point, °C	81
Boiling point, °C	222
Log octanol/water coefficient, log Pow	-1.26 (Sangster 1989)
LD50 values to mammals in oral exposure, mg/kg	7000 orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	2300 unk-rat (Lewis & Sweet 1984)
Carcinogenicity	Carcinogenicity: weak (Verschueren 1983).
Mutagenicity	Mutagenicity in the Salmonella test: neg. < 0.0008 revertant colonies/nmol; < 70 revertant colonies at 5000 µg/plate (Verschueren 1983).
LD50 values to birds in oral exposure, mg/kg	> 101 orl-Agelaius phoeniceus (Schafer et al. 1983)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): > 10000 mg/l (Bringmann & Kühn 1980a)
LOEC values to algae, mg/l	6200 rpd, act, Microcystis aeruginosa, Bringmann & Kühn 1976
LC50 values to fishes, mg/l	1550–2000 Gambusia affinis (Meinck et al. 1970)
Other information about water organisms	LOEC 6200 mg/l, rpd, act, Microcystis aeruginosa (Bringmann & Kühn 1980a). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): > 10000 mg/l protozoa (Entosiphon sulcatum): 99 mg/l (Bringmann & Kühn 1980a)

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9 • Acetanilide

103-84-4

Synonyms	N-Phenylacetamide Antifebrin N-Phenylethanamide	
Sumformula of the chemical	C8H9NO	
Use	Stabilizer for cellulose ester coatings.	
Odour	Odour threshold: 270 mg/m³	
Molecular weight	135.16	
Specific gravity (water=1)	1.21	at 4/4 °C
Water solubility, mg/l	5630 1000	25 °C 189 ml 6 °C (MITI 1992)
Melting point, °C	113–114	(MITI 1992)
Boiling point, °C	304	760 mmHg (MITI 1992)
Log octanol/water coefficient, log Pow	0.95 1.16	Anon. 1986 (Sangster 1989)
Log soil sorption coefficient, log Kom	1.19	(Sabljic 1987)
Total degradation in water	Biodegradation: 68.7 by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
Other information about mammals	Rats, monkeys tolerated oral doses of 200–400 mg/kg for many weeks (Patty 1967).	
LD50 values to birds in oral exposure, mg/kg	> 100 > 100	orl-Agelaius phoeniceus orl-Sturnus vulgaris (Schafer et al. 1983)
LC50 values to fishes, mg/l	100 115	96 hr, Lepomis macrochirus 96 hr, Menidia audens (Gaynor et al. 1975)

10 • Acetic acid

64-19-7

Synonyms	Ethanoic acid Methanecarboxylic acid Glacial acetic acid Vinegar acid
Sumformula of the chemical	CH3COOH
Use	Manufacturing source: beetsugar manufacturing; winery; vinegar manufacturing; textile mills; wood distillation plants. Users and formulation: food processing plants; organic chemical manufacturing; nylon and fibre manufacturing; dyestuff and pigments manufacturing; vitamins, antibiotics, hormones manufacturing; rubber manufacturing; photographic chemicals manufacturing; ester solvents manufacturing; plastic manufacturing. Natural sources: both plants and animals as normal metabolite. Man caused sources: domestic use of vinegar; photographic film developing; lab use (EPA 1975).

State and appearance	Colourless liquid.	
Odour	Characteristic, sour, pungent. Odour index: 15000 (Verschueren 1983)	
Molecular weight	60.05	
Specific gravity (water=1)	1.049	at 20/4 °C
Vapour density (air=1)	2.1	
Conversion factor, 1 ppm in air=	2.494	mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.401	ppm
Vapour pressure, mmHg	11.4 20 12	20 °C 30 °C 20 °C (Weber et al. 1981)
Water solubility, mg/l	6029	at 25 °C (Yalkowsky et al. 1987)
Melting point, °C	16.6	
Boiling point, °C	117.9 118.5	
pKa	4.75 4.76	at 25 °C (West 1985) (Sangster 1989)
Log octanol/water coefficient, log Pow	-0.31 -0.17 -0.17	 (Hansch & Leo 1985) (Sangster 1989)
Henry's law constant, Pa x m^3/mol	0.0101325 at pH 4 (Gaffney et al. 1987) 0.0001013 at pH 7 (Gaffney et al. 1987) 0.1211 calc. (Yaws et al. 1991)	
Volatilization	The values of Henry's law constant at various pH's indicates that acetic acid will not volatilise significantly from water (Lyman et al. 1982).	
Mobility	In 24 hr aqueous adsorption studies using montmorillite and kaolinite clay adsorbents, 2.4–30.4% of added acetic acid was observed to be in the adsorbed phase (Hemphill & Swanson 1964). In adsorption studies using the adsorbent hydroxyapatite, only 5% of added acetic acid became adsorbed to the hydroxyapatite (Gordon & Millero 1985).	
Total degradation in soil	A large number of biological screening studies have determined that acetic acid biodegrades readily under both aerobic and anaerobic conditions. Acetic acid has been noted to leach from biological disposal areas; however, it is expected to be efficiently biodegraded during its migration through soil (Abrams et al. 1975).	
Total degradation in water	The dominant environmental fate process for acetic acid in water is biodegradation. A large number of biological screening studies have determined that acetic acid biodegrades readily under both aerobic and anaerobic conditions. Aquatic hydrolysis and bioconcentration are not important. Two aqueous adsorption studies found that acetic acid exists primarily in the water column (Howard II 1990).	

Other information about degradation	Warburg respirometer, 30-day 60% BODT, acclimated sewage seed (Helfgott et al. 1977). AFNOR T 90/103 test, 5-day 36% BODT, microbes from 3 polluted surface waters (Dore et al. 1975). Standard dilution BOD water, 5-day 57.7% BODT avg (Heukelekian & Rand 1955). Seawater dilution, 66-100% BODT in 5–20 days, sewage inocula (Price et al. 1974). Warburg respirometer, 5-day 77% BODT, sewage inocula (Dias & Alexander 1971). Standard dilution BOD water, 5-day 81.3% BODT; seawater dilution, 5-day 77.6% bodt (Takemoto et al. 1981). Standard dilution BOD water, 5-day 63.2% BODT, sewage inocula (Saito et al. 1984).		
Metabolism in mammals	May be absorbed into the body by inhalation and ingestion.		
Other information about bioaccumulation	Based on the log Kow, the BCF for acetic acid can be estimated to be less than 1. This indicates that bioconcentration is not significant (Lyman et al. 1982).		
LD50 values to mammals in oral exposure, mg/kg	3300	orl-mam (Patty 1967)	
LC50 values to mammals in inhalation exposure, ppm	5000	1 hr, ihl-mus, gpg (Patty 1967)	
Health effects	Man:	severe toxic effects: symptoms of illness: unsatisfactory: (Verschueren 1983).	200 ppm = 500 mg/m³, 60 min 40 ppm = 100 mg/m³, 60 min. 20 ppm = 50 mg/m³
	Corrosive to the eyes, the skin and the respiratory tract. Inhalation of vapour and/or fumes may cause shortness of breath (lung oedema). Serious cases may be fatal.		
Carcinogenicity	Carcinogenicity: none (Verschueren 1983).		
Mutagenicity	Mutagenicity in the Salmonella test:none (Verschueren 1983).		
Effects on plants	Phytotoxity: EC50 * mg/m³		
	wheat alfalfa tobacco soybean corn (Thompson et al. 1979)	23.3 7.8 41.2 20.1 50.1	** EC50 = concentration required to cause visible injury in 50% of the leaves of the plant population exposed for a 2 hr fumigation period.*
Maximum longterm immission concentration in air for plants, mg/m³	5	VDI 2306	
Maximum longterm immission concentration in air for plants,ppm	2	VDI 2306	
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 2850 mg/l (Bringmann & Kühn 1980a).		
LOEC values to algae, mg/l	90 4000	rpd, act, Microcystis aeruginosa (Bringmann & Kühn 1976) rpd, act, Scenedesmus quadricauda (Bringmann & Kühn 1980a)	
LC50 values to crustaceans, mg/l	47	24 hr, Daphnia magna (Elkins et al. 1956)	
LC50 values to fishes, mg/l	88 75	96 hr, Pimephales promelas (Vincent et al. 1976) 96 hr, Lepomis macrochirus (Price et al. 1974)	

Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): algae (Microcystis aeruginosa): 90 mg/l; green algae (Scenedesmus quadricauda): 4000 mg/l; protozoa (Entosiphon sulcatum): 78 mg/l; protozoa (Uronema parduczi): 1350 mg/l (Verschueren 1983).

11 • Acetic anhydride

108-24-7

Synonyms	Acetic oxide Acetyl oxide Ethanoic anhydride Acetic acid, anhydride Acetyl anhydride Acetyl ether	
Sumformula of the chemical	C4H6O3	
State and appearance	Colourless liquid.	
Odour	Characteristic, sour acid, neutral to pleasant. Threshold odour concentration: 50% recognition: 0.36 ppm 100% recognition: 0.36 ppm Odour index: 14 611 (Verschueren 1983) Quality: sour acid Hedonic tone: neutral to unpleasant Threshold odour concentration: absolute: < 0.14 ppm 50% recognition: 0.36 ppm 100% recognition: 0.36 ppm Odour index 100% recognition: 14 611 (Hellman & Small 1974).	
Molecular weight	102.09	
Specific gravity (water=1)	1.083	at 20/20 °C
Conversion factor, 1 ppm in air=	4.24	mg/m³
Conversion factor, 1 mg/m³ in air=	0.236	ppm
Vapour pressure, mmHg	3.5 5 7	20 °C 25 °C 30 °C
Melting point, °C	-68– -73	
Boiling point, °C	139.9	
LD50 values to mammals in oral exposure, mg/kg	1780	orl-rat (Patty 1967)
LD50 values to mammals in non-oral exposure, mg/kg	4000	skn-rbt (Sweet 1987)
LC50 values to mammals in inhalation exposure, ppm	1000	ihl-rat, 4 hr (Sweet 1987)

Other information about mammals	Skin and eye irritation: skin, rabbit, 10 mg, 24 hr open, mild; skin, rabbit, 540 mg open, mild; eye, rabbit, 0.250 mg open, severe (Sweet 1987).
Health effects	Man: severe eye and skin irritant (Verschueren 1983)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 1150 mg/l (Bringmann & Kühn 1980a)
EC50 values to algae, mg/l	360 srv, act, Chlorella pyrenoidosa (Jones 1971)
LOEC values to algae, mg/l	3400 rpd, act, Scenedesmus quadricauda (Bringmann & Kuhn 1980a)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 3400 mg/l protozoa (Entosiphon sulcatum): 30 mg/l (Bringmann & Kühn 1980a)

12 • N-Acetoacetyl-2-methyl aniline 93-68-5

Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

13 • Acetone 67-64-1

Synonyms	2-Propanone
Sumformula of the chemical	CH3-CO-CH3
Use	Manufacture of smokeless powder; paints, varnishes, lacquers manufacturing; organic chemicals manufacturing; pharmaceuticals manufacturing; sealants and adhesives manufacturing; solvents for celluloses acetate, nitrocellulose, acetylene. Natural sources: normal micro component in blood and urine; minor constituent in pyroligneous acid; oxidation of alcohols and humic substances (EPA 1975).
State and appearance	Clear colourless liquid.
Odour	Characteristic, sweet, fruity, pleasant to neutral. Odour index: 1740 Threshold for unadapted persons: 0.03% in diluent Threshold after adaption with pure odourant: 5.0% in diluent (Verschueren 1983). USSR: Human odour perception: non perception: 0.8 mg/m³ perception: 1.1 mg/m³ Animal chronic exposure: no effect: 0.5 mg/m³ Human reflex response: no response: 0.35 mg/m³ adverse response: 0.55 mg/m³ (Stern 1968) Quality: sweet, fruity Hedonic tone: pleasant to neutral Threshold odour concentration: absolute: 20.0 ppm 50% recognition: 32.5 ppm 100% recognition: 140 ppm Odour index 100% recognition: 1 742 (Hellman & Small 1974).
Molecular weight	58.09

Aceton

Specific gravity (water=1)	0.791	20 °C
Conversion factor, 1 ppm in air=	2.411	mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.415	ppm
Vapour pressure, mmHg	270 231	30 °C 25 °C (Buttery et al. 1969)
Melting point, °C	-95 -95.35	
Boiling point, °C	56.2	at 760 mmHg
Log octanol/water coefficient, log Pow	-0.24 -0.24	(Hansch & Leo 1985) (Sangster 1989)
Henry's law constant, Pa x m^3/mol	3.72 4.333	(Snider & Dawson 1985) calc. (Yaws et al. 1991)
Volatilization	Relative volatility (nBuAc=1) = 14.48 Acetone has a high vapour pressure and low adsorption to soil and should therefore readily evaporate from the soil surface. When a variety of moist soils were treated with acetone and the head space analysed over the course of 3 days, acetone was found in the air above all samples (Pavlica et al. 1978).	
Adsorption/desorption	Acetone's miscibility in water would suggest that it does not adsorb appreciably to soil (Lyman et al. 1982). It displayed no adsorption to montmorillonite or kaolinite clay or stream sediment (Rathbun et al. 1982) (Wolfe et al. 1986).	
Photochemical degradation in water	No photo degradation occurred when acetone was exposed to sunlight for 23 hr in distilled water or 15 hr in stream water (Rathbun et al. 1982).	
Chemical oxygen demand, g 02/g	1.92	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	1.85	5 days (Bridie et al. 1979)
Total degradation in soil	Acetone will both volatilize and leach into the ground. Acetone readily biodegrades and there is evidence suggesting that it biodegrades fairly rapidly in soils (Howard II 1990).	
Total degradation in water	Acetone is readily biodegradable in screening tests, although data from natural water are lacking. It will also be lost due to volatilization (estimated half-life 20 hr from a model river). Adsorption to sediment should not be significant (Howard II 1990).	
Other information about degradation	Impact on biodegradation processes: Digestion on sludge is inhibited from 4 g/l. Nitrification of activated sludge is decreased with 75% at 840 mg/l (Meinck et al.1970). Slight inhibition of microbial growth after 24 hr exposure at 5 ppm (Verschueren 1983). Approximately 50% inhibition of ammonia oxidation in Nitrosomonas at 8100 mg/l (Hooper & Terry 1973). Acetone readily biodegrades in screening tests. Typical results using sewage inocula are: 54% theoretical BOD after 5 days (Bridie et al. 1979) 71% theoretical BOD in 7 days (Helfgott et al. 1977) 38% theoretical BOD in 5 days (Vaishnav et al. 1987) 56% and 38% theoretical BOD after 5 days and 84% and 76% theoretical BOD after 20 days in fresh and salt water, respectively (Price et al. 1974) Acetone also degrades under anaerobic conditions, with one investigator reporting 100% degradation in 4 days after a 5 day lag (Chou et al. 1979)	

Other information about bioaccumulation	Using the recommended log octanol/water partition coefficient, the potential for acetone bioconcentration in fish is negligible. (Lyman et al. 1982) One experimental study of bioconcentration in adult haddock at 7–9 °C (static test) resulted in a BCF of 0.69. (Howard II 1990)	
LD50 values to mammals in oral exposure, mg/kg	7400 3000	orl-rat orl-mus (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	20000	skn-rbt (Lewis & Sweet 1984)
LCLo values to mammals in inhalation exposure, ppm	1600	4 hr, ihl-rat (Lewis & Sweet 1984)
TCLo values to mammals in inhalation exposure, mg/kg	0.44	6 min., ihl-man (Lewis & Sweet 1984)
Health effects	Man: repeated exposure to 25–920 ppm: chronic conjunctivitis, pharyngitis, bronchitis, gastritis, gastroduodenitis. Light irritation of the mucous membrane above 300 ppm. Severe toxic effects: 4000 ppm = 9659 mg/m³, 60 min. Symptoms of illness: 800 ppm = 1930 mg/m³, 60 min. Unsatisfactory:> 400 ppm = 965 mg/m³, 60 min. Estimated minimum lethal dose by ingestion: 50 ml. (Verschueren 1983)	
Carcinogenicity	Carcinogenicity: none (Verschueren 1983).	
Mutagenicity	Mutagenicity in the salmonella test: none (Verschueren 1983).	
Effects on amphibia	Mexican axoloth (3–4) w after hatching): 48 hr, LC50: 20000 mg/l Clawed toad (3–4) w after hatching): 48 hr LC50: 24000 mg/l (Slooff & Baerselman 1980).	
Maximum longterm immission concentration in air for plants,mg/m³	120	VDI 2306
Maximum longterm immission concentration in air for plants,ppm	50	VDI 2306
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 1700 mg/l (Bringmann & Kühn 1980a)	
EC50 values to microorganism, mg/l	16000 594 21000 35545	Microtox (Tarkpea et al. 1986) 6 hr Growth P. putida (Slabbert 1986) 15 min Microtox (Hermens et al. 1985) Biodegradation inhibition (Vaishnav 1986)
LOEC values to algae, mg/l	530 7500	rpd, act, Microcystis aeruginosa (Bringmann & Kühn 1976) rpd, act, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
LC50 values to crustaceans, mg/l	12700 8800 7635 16700 7550 6000	48 hr, Daphnia magna 48 hr, Daphnia pulex 48 hr, Daphnia cucullata (Canton & Adema 1978) 96 hr, 10 °C, Nitocra spinipes (Linden et al. 1979) 48 hr, Asellus aquaticus (Slooff 1983) 48 hr, Gammarus pulex (Slooff 1983)

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LC50 values to fishes, mg/l	5000	24 hr, Carassius auratus (Anon.1975)
	6100	24 hr, Salmo trutta (Majewski et al.1978)
	7032	14 d, Poecilia reticulata (Klnemann 1979)
	7280–8140	Pimephales promelas (Veith et al.1983)
	11000	96 hr, 10 °C, Alburnus alburnus (Linden et al. 1979)
Other information about water organisms	LOEC 28 mg/l, rpd, act, Entosiphon sulcatum (Bringmann & Kühn 1980a). EC50, growth, 10 days, 0.36%, Anabaena cylindrica EC50, growth, 10 days, 2.75%, Anabaena inaequalis EC50, growth, 10 days, 0.56%, Anabaena sp. EC50, growth, 10 days, 3.69%, Anabaena variabilis EC50, growth, 10 days, 4.38%, Nostoc sp. (Stratton 1987). LC50, 48 hr, 15000 mg/l, Tubificidae LC50, 48 hr, 13000 mg/l, Chironomus gr. thummi LC50, 48 hr, 7000 mg/l, Erpobdella octoculata LC50, 48 hr, 7000 mg/l, Lymnaea stagnalis LC50, 48 hr, 7500 mg/l, Dugesia cf. lugubris LC50, 48 hr, 13500 mg/l, Hydra oligactis LC50, 48 hr, 5000 mg/l, Corixa punctata LC50, 48 hr, 6400 mg/l, Ischura elegans LC50, 48 hr, 10300 mg/l, Nemoura cinerea LC50, 48 hr, 7600 mg/l, Cloeon dipterum (Slooff 1983) Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 7500 mg/l protozoa (Entosiphon sulcatum): 28 mg/l (Bringmann & Kühn 1980a)	

14 • Acetonitrile 75-05-8

Synonyms	Methylcyanide Ethanenitrile	
Sumformula of the chemical	CH3CN	
Use	Solvent; manufacture of synthetic pharmaceuticals.	
State and appearance	Colourless liquid	
Odour	Threshold Odour Concentration: 68 mg/m³ (39.8 ppm); detection: 1950 mg/m³ (Verschueren 1983).	
Molecular weight	41.05	
Specific gravity (water=1)	0.79	at 20/4 °C
Vapour density (air=1)	1.42	
Conversion factor, 1 ppm in air=	1.706	mg/m³
Conversion factor, 1 mg/m³ in air=	0.586	
Vapour pressure, mmHg	74	20 °C
Melting point, °C	-44	
Boiling point, °C	82	
Log octanol/water coefficient, log Pow	-0.34	(Sangster 1989)

Henry's law constant, Pa x m³/mol	2.033 calc. (Yaws et al. 1991)
Volatilization	Relative volatility (nBuAc=1) = 4.55
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
Other information about degradation	Biodegradation by mutant microorganisms (Verschueren 1983) - 500 mg/l at 20 °C % disruption: parent: 100% in 9 hr; mutant: 100% in 1.5 hr
LD50 values to mammals in oral exposure, mg/kg	1700–8500 orl-rat 180 orl-gpg (Verschueren 1983) 3800 rat 177 gpg (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	1250 skn-rbt (Lewis & Sweet 1984)
LC50 values to mammals in inhalation exposure, ppm	7500 8 hr, ihl-rat (Verschueren 1983)
LCLo values to mammals in inhalation exposure, ppm	8000 4 hr, ihl-rat (Lewis & Sweet 1984)
TDLo values to mammals in oral exposure, mg/kg	570 orl-hmn (Lewis & Sweet 1984)
Health effects	Man: no specific response: 160 ppm, 4 hr (Verschueren 1983).
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): Bacteria (Pseudomonas putida): 680 mg/l Protozoa (Uronema parduczi): 5825 mg/l (Verschueren 1983).
LOEC values to algae, mg/l	520 rpd, act, Microcystis aeruginosa (Bringmann & Kuhn 1976) 7300 rpd, act, Scenedesmus quadricauda (Bringmann & Kuhn 1980a)
LC50 values to fishes, mg/l	1000 96 hr, Pimephales promelas 1650 96 hr, Poecilia reticulata (Jones 1971)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 7300 mg/l protozoa (Entosiphon sulcatum): 1810 mg/l (Bringmann & Kühn 1980a)

15 • Acetophenone 98-86-2

Synonyms	Methylphenylketone Hypnone Acetylbenzene Phenylmethylketone
Sumformula of the chemical	C8H8O
Use	Manufacturing source: organic chemical industry: coal processing industry. Uses and formulation: perfume manufacturing; solvent for synthesis of pharmaceuticals, rubber, chemicals, dyestuffs and corrosion inhibitors; plasticizer manufacturing; tobacco flavourant; intermediate in synthesis of pharmaceuticals. Natural sources (water and air): oils of castoreum and labdanum resin; buds of balsam poplar; heavy oil fraction of coal tar. Manmade sources: in gasoline exhaust: < 0.1 to 0.4 ppm

State and appearance	Colourless liquid.
Odour	Sweet almond, pleasant. Threshold Odour Concentration: 0.01 mg/m³ = 2 ppb; average: 0.17 ppm, range: 0.0039 to 2.02,17 panellists; absolute perception limit: 0.30 ppm; 50% recognition: 0.60 ppm; 100% recognition: 0.60 ppm; Odour index: 2183 USSR: human odour perception: 0.01 mg/m³ human reflex response: no response: 0.003 mg/m³ adverse response: 0.007 mg/m³ animal chronic exposure: adverse effect: 0.07 mg/m³ (Verschueren 1983). Quality: sweet, almond Hedonic tone: pleasant Threshold odour concentration absolute: 0.30 ppm 50% recognition: 0.60 ppm 100% recognition: 0.60 ppm Odour index 100% recognition: 2 183 (Hellman & Small 1974).
Molecular weight	120.1
Specific gravity (water=1)	1.03 at 20/4 °C
Vapour density (air=1)	4.14
Conversion factor, 1 ppm in air=	4.99 mg/m³
Conversion factor, 1 mg/m³ in air=	0.2 ppm
Vapour pressure, mmHg	1 15 °C
Water solubility, mg/l	5500
Melting point, °C	19
Boiling point, °C	202
Log octanol/water coefficient, log Pow	1.73 (Anon. 1986) 1.59 (Schwarzenbach & Westall 1981) 1.63 (Sangster 1989)
Log organic C/water coefficient, log Pcw	1.63 exptl (Schwarzenbach & Westall 1981) 1.63 calcd (Schwarzenbach & Westall 1981)
Log soil sorption coefficient, log Kom	1.63 (Sabljic 1987)
Total degradation in water	Biodegradation: 64.7% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992)
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
EC50 values to microorganism, mg/l	1922 Biodegradation inhibition (Vaishnav 1986)
LC50 values to fishes, mg/l	155 96 hr, Pimephales promelas (Verschueren 1983) 236 96 hr, Pimephales promelas (Broderius & Kahl 1985)

Other information about water organisms	Taste in fish: 0.5 mg/l (Verschueren 1983).

16 • Acetoxime 127-06-0

Synonyms	2-Propanoneoxime Acetoneoxime
Sumformula of the chemical	(CH3)2CNOH
Use	Organic synthesis (intermediate); solvent.
Molecular weight	73.09
Specific gravity (water=1)	0.97 20/20 °C
Melting point, °C	61
Boiling point, °C	136.3
Effects on microorganisms	Pseudomonas: toxic at 0.3 g/l (Verschueren 1983).

17 • Acetyl bromide 506-96-7

LC50 values to fishes, mg/l	40.6	96 hr, Pimephales promelas (Curtis & Ward 1981)

18 • Acetyl chloride 75-36-5

LC50 values to fishes, mg/l	42	96 hr, Pimephales promelas (Curtis & Ward 1981)

19 • Acetyl tributylcitrate 77-90-7

Sumformula of the chemical	C20H34O8
EINECS-number	2010670
Water solubility, mg/l	5 (MITI 1992)
Boiling point, °C	173 (MITI 1992)
Total degradation in water	Biodegradation: 82% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).

20 • N-Acetyl-4-ethoxyaniline 62-44-2

Melting point, °C	134.8–135.6 (MITI 1992)
Total degradation in water	Biodegradation: 8.4% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

Bioconcentration factor, fishes	< 3 < 30	6w, Cyprinus carpio, conc 0.3 mg/l 6w, Cyprinus carpio, conc 0.03 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	335	48hr, Oryzias latipes (MITI 1992)

21 • 2-Acetylaminofluorene 53-96-3

Effects on the physiology of water organisms	Biochemical effect (change in physiochemical process including glycogen uptake, cholesterol levels and lipid analysis): 0.63 mmol, Salmo gairdneri, 6 days (Miyauchi & Uematsu 1987).

22 • Acetylcyclohexyl methylcyclohexylamine 53710-61-5

Other information about mammals	LDfr = 36.6 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

23 • Acetylene 74-86-2

Synonyms	Ethine Ethyne	
Sumformula of the chemical	CHCH	
Use	Manmade sources: Diesel engine: 14.1% of emitted hydrocarbons Reciprocating gasoline engine: 3.3% of emitted hydrocarbons Rotary gasoline engine: 3.3% of emitted hydrocarbons (Verschueren 1983).	
State and appearance	Colourless gas.	
Odour	Odour threshold: detection: 240 mg/m³; 1300–2750 mg/m³ (Verschueren 1983)	
Molecular weight	26.04	
Specific gravity (water=1)	0.62	liquified
Vapour density (air=1)	0.91	
Conversion factor, 1 ppm in air=	1.08	mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.92	ppm
Melting point, °C	-81.8	
Sublimation point, °C	-84	
Henry's law constant, Pa x m^3/mol	2557	calc. (Yaws et al. 1991)
Other reactions in atmosphere	Atmospheric reactions: reactivity; NO ox.: ranking: 0.1 (Verschueren 1983).	
Effects on plants	Seed plants: sweet pea: declination in seedling: 250 ppm, 3 days – tomato: epinasty in petiole: 50 ppm, 2 days (Verschueren 1983).	
LC50 values to fishes, mg/l	200	33 hr, Salmo trutta (Meinck et al. 1970)

24 • Acetylenetetrabromide 79-27-6

Synonyms	1,1,2,2-Tetrabromoethane sym-Tetrabromoethane	
Sumformula of the chemical	CHBr2-CHBr2	
State and appearance	Colourless to yellow liquid.	
Molecular weight	345.7	
Specific gravity (water=1)	2.964	
Vapour density (air=1)	11.9	
Conversion factor, 1 ppm in air=	14.37	mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.07	ppm
Vapour pressure, mmHg	0.1	20 °C
Water solubility, mg/l	651	30 °C
Melting point, °C	0.1 -20	 (MITI 1992)
Boiling point, °C	239–242	(MITI 1992)
Total degradation in water	Biodegradation: 29.0% by BOD period: 12d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	0.5–7.0 < 2.9–8.2	6w, Cyprinus carpio, conc 10 000 mg/l 6w, Cyprinus carpio, conc 1000 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	400	orl-rbt, gpg (Verschueren 1983)
Other information about mammals	Rats, guinea pigs, monkey: growth depression in guinea pigs, all animals increase liver weight: 14 ppm, 7 hr/days, 5days/w, 100 to 106 days (Verschueren 1983). Rat; single oral dose: survived; 600 mg/kg Rat; single oral dose: succumbed 1600 mg/kg (Verschueren 1983).	
LC50 values to fishes, mg/l	19	48 hr, Oryzias latipes (MITI 1992)

25 • N-Acetylglycine 543-24-8

Synonyms	N-Acetyl-2-aminoethanoic acid Aceturic acid Acetamido acetic acid Acetylamino acetic acid	
Sumformula of the chemical	CH3CONHCH2COOH	
Use	Medicine	
Molecular weight	117.1	
Water solubility, mg/l	21700	at 15 °C

Melting point, °C	206
Log octanol/water coefficient, log Pow	-1.8

26 • 1-Acetylnaphthalene

941-98-0

Effects on arthropods	LC50, 1 day, 10 mg/l, Aades aegypti LC50, 1 day, > 10 mg/l, Aades taeniorhynchus LC50, 1 day, 6.46 mg/l, Culex quinquefasciatus (Borovsky et al. 1987).

27 • 2-Acetylnaphthalene

93-08-3

Effects on arthropods	LC50, 1 day, 2.37 mg/l, Aades aegypti LC50, 1 day, 7.80 mg/l, Aades taeniorhynchus LC50, 1 day, 4.64 mg/l, Culex quinquefasciatus (Borovsky et al. 1987).

28 • 3-Acetyloxolane-2-one

517-23-7

Sumformula of the chemical	C6H8O3
Total degradation in water	Biodegradation: 72.0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

29 • 4-Acetylpyridine

1122-54-9

Sumformula of the chemical	C7H7NO	
Log octanol/water coefficient, log Pow	0.5	(Anon. 1986)
LD50 values to birds in oral exposure, mg/kg	100–750	orl-Agelaius phoeniceus (Schafer et al. 1983)

30 • 1-Acetylthiourea

591-08-2

Other information about mammals	ALD = 94.0 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987).	
LD50 values to birds in oral exposure, mg/kg	> 96	orl-Agelaius phoeniceus (Schafer et al. 1983)

31 • Acid Blue 45

2861-02-1

Sumformula of the chemical	C14H8N2O10S2.2Na	
Water solubility, mg/l	780	(MITI 1992)
Melting point, °C	> 300	(MITI 1992)

Total degradation in water	Biodegradation: 2–4% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.09–0.3 < 0.9–3.2	6w, Cyprinus carpio, conc 1 mg/l 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 350	48 hr, Oryzias latipes (MITI 1992)

32 • Acid Red 114 6459-94-5

Water solubility, mg/l	> 500	(MITI 1992)
Bioconcentration factor, fishes	42–76 52–84	8w, Cyprinus carpio, conc 0.2 mg/l 8w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	4	48 hr, Oryzias latipes (MITI 1992)

33 • Acid yellow 23 1934-21-0

Water solubility, mg/l	> 20000	(MITI 1992)
Bioconcentration factor, fishes	< 0.29 < 3.0	6w, Cyprinus carpio, conc 0.6 mg/l 6w, Cyprinus carpio, conc 0.06 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	> 1000	48 hr, Oryzias latipes (MITI 1992)

34 • Acreoline-HBr 300-08-3

Other information about mammals	ALD = 80.0 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987).

35 • Acridine 260-94-6

Sumformula of the chemical	C13H9N	
Use	Manufacturing source: coal tar. Use: Manufacturing of dyes.	
State and appearance	Small, colourless needles	
Molecular weight	179.21	
Specific gravity (water=1)	1.1	20/4 °C
Melting point, °C	108	
Boiling point, °C	346	
Sublimation point, °C	100	

pKa	10.65	(Sangster 1989)
Log octanol/water coefficient, log Pow	3.4	(Sangster 1989)
Log soil sorption coefficient, log Kom	4.22 4.26	observed (Sabljic 1987) calculated (Sabljic 1987)
Bioconcentration factor, fishes	127 874	Pimephales promelas (Verschueren 1983) P. promelas, uptake via interaction with contaminated sediment
Bioconcentration factor, crustaceans	29.6	Daphnia pulex (Verschueren 1983)
LD50 values to mammals in non-oral exposure, mg/kg	100	ivn-rbt (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	> 101	orl-Agelaius phoeniceus (Schafer et al. 1983)
EC50 values to algae, mg/l	20	4 hr, pht, Selenastrum capricornutum (Millemann et al. 1984)
NOEC values to algae, mg/l	0.3	rpd, chr, Diaptomus clavipes (Cooney & Gehrs 1985)
LC50 values to crustaceans, mg/l	2.9 2.1 2.92	24 hr, Daphnia pulex (Southworth et al. 1978) 48 hr, Daphnia magna (Millemann et al. 1984) 24 hr, Daphnia pulex (Verschueren 1983)
LC50 values to fishes, mg/l	0.3 0.44 0.32 10.05 1.02	27 days, Salmo gairdneri (Millemann et al. 1984) 0d, embryo-larval, Salmo gairdneri 4d, embryo-larval, Salmo gairdneri 0d, embryo-larval, Micropterus salmoides 4d, embryo-larval, Micropterus salmoides (Black et al. 1983)
Other information about water organisms	Inhibition of photosynthesis of a freshwater, non-axenic uni-algal culture of Selenastrum capricornutum at 1% saturation; 92% carbon-14 fixation (vs. controls) 10% saturation; 75% carbon-14 fixation (vs. controls) 100% saturation; 1% carbon-14 fixation (vs. controls) (Verschueren 1983). Lethal threshold concentration: 0.4401 mg/l, 0.04 days, Daphnia magna (Newsted & Giesy 1987) 0.525 mg/l, 0.18 days, Pimephales promelas (Oris et al. 1987).	

36 • Acrolein

107-02-8

Synonyms	Acryl aldehyde Allyl aldehyde 2-Propenal
Sumformula of the chemical	C3H4O
Known impurities	Hydrochinon * 0.1% m (w) to prevent polymerisation
State and appearance	Colourless to yellowish liquid
Odour	Characteristic. Quality: burnt sweet, hot fat, acrid. Hedonic tone; pungent. (Verschueren 1983). Human odour perception; 0.8 mg/m³ Human reflex response: adverse response; 0.6 mg/m³ Animal chronic exposure; adverse effect; 0.15 mg/m³ (Verschueren 1983). Odour threshold: 0.11 mg/kg (Verschueren 1983).

Molecular weight	56.07	
Specific gravity (water=1)	0.8427	at 20/20 °C
Vapour density (air=1)	1.94	
Conversion factor, 1 ppm in air=	2.328	mg/m³
Conversion factor, 1 mg/m³ in air=	0.43	ppm
Vapour pressure, mmHg	220	20 °C
Water solubility, mg/l	208000	
Melting point, °C	-87.7	
Boiling point, °C	52.5	
Log octanol/water coefficient, log Pow	-0.01	(Sangster 1989)
Chemical oxygen demand, g 02/g	1.72	5 days (Bridie et al. 1979)
Other information about degradation	BOD, 5 days, 0.00 g 02/g. (Bridie et al. 1979)	
LD50 values to mammals in oral exposure, mg/kg	46 7	orl-rat orl-rbt (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	562	skn-rbt (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	10.0–100 10.0–100	orl-Agelaius phoeniceus orl-Sturnus vulgaris (Schafer et al. 1983)
Effects on arthropods	Insects: mayfly nymphs (Ephemerella walkeri): lowest observed avoidance concentration > 0.1 mg/l. Tanytarsus dissimilis: LC50, 2 days, > 0.151 mg/l (Holcombe et al. 1987).	
Maximum longterm immission concentration in air for plants, mg/m³	0.01	VDI 2306
Maximum longterm immission concentration in air for plants, ppm	0.005	VDI 2306
Effects on microorganisms	Bacteria: Pseudomonas putida: inhibition fo cell multiplication starts at 0.21 mg/l (Verschueren 1983).	
LOEC values to algae, mg/l	0.04	rpd, act, Microcystis aeruginosa (Bringmann & Kuhn 1976)
LC50 values to crustaceans, mg/l	0.083	48 hr, Daphnia magna (LeBlanc 1980)
EC50 values to crustaceans, mg/l	0.051	mbt, 2d, Daphnia magna (Holcombe et al. 1987)
NOEC values to crustaceans, mg/l	0.026	rpd, schr, Daphnia magna (Macek et al. 1976c)

LC50 values to fishes, mg/l	0.08	24 hr, Lepomis macrochirus (Bond et al. 1960)
	0.046 0.079	24 hr, Salmo trutta lacustris 24 hr, Lepomis macrochirus (Burdick et al. 1964)
	0.08	24 hr, Carassius auratus (Anon. 1975)
	0.09	96 hr, L epomis macrochirus (Buffafusco et al. 1981)
	0.08 0.07	96 hr, Salmo gairdneri 96 hr, Lepomis macrochirus (Foster 1981)
	0.014 0.033 0.014 0.016	4d, Catostomus commersoni 4d, Lepomis macrochirus 4d, Pimephales promelas 4d, Salmo gairdneri (Holcombe et al. 1987)
	0.029	4d, Salmo gairdneri (McKim et al. 1987)
	0.02	4d, Pimephales promelas (Geiger et al. 1988)
LOEC values to fishes, mg/l	0.042	srv, chr, Pimephales promelas (Macek et al. 1976c)
NOEC values to fishes, mg/l	0.011 0.026	srv, chr, Pimephales promelas rpd, chr, Pimephales promelas (Macek et al. 1976c)
Other information about water organisms	Algae: Microcystis aeruginosa: inhibition of cell multiplication starts at 0.04 mg/l (Verschueren 1983). Fishes: rainbow trout (Salmo gairdneri): lowest observed avoidance concentration 0.1 mg/l (Verschueren 1983). Salmo gairdneri: Lethal threshold concentration: 0.07698 mg/l, 0.85 days (McKim et al. 1987). LC50, 4d, > 0.151 mg/l, Aplexa hypnorum (Holcombe et al. 1987).	
Other information	Manmade sources: in cigarette smoke; 150 ppm; in gasoline exhaust: 0.2 to 5.3 ppm; 2.6–9.8 vol. % of total exhaust aldehydes (Verschueren 1983). Experimental concentrations of 0.1 mg/l can significantly taint the flesh of rainbow trouts to make them unpalatable (Verschueren 1983).	

37 • Acrylamide

79-06-1

Synonyms	Propenamide Acrylic amide	
Sumformula of the chemical	CH2=CHCONH2	
Use	Synthesis of dyes; polymers or copolymers as plastics, adhesives, soil conditioning agents; flocculants.	
Molecular weight	71.08	
Vapour density (air=1)	2.46	
Conversion factor, 1 ppm in air=	2.95	mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.34	ppm
Vapour pressure, mmHg	2 10	at 87 °C at 117 °C
Water solubility, mg/l	2050000	

Melting point, °C	84–85	
Log octanol/water coefficient, log Pow	-0.78	(Sangster 1989)
Chemical oxygen demand, g 02/g	1.33	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.05 0.92	5 days (Bridie et al. 1979) 5 days, seeding adapted
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LC50 values to fishes, mg/l	400	48 hr, Salmo trutta m. lacustris (Woodiwiss & Fretwell 1974)
	130	96 hr, Rasbora heteromorpha (Tooby et al. 1975)
	460 160	24 hr, Carassius auratus 96 hr (Bridie et al. 1979)
	350	14d, Poecilia reticulata (Hermens & Leeuwangh 1982)
Effects on the physiology of water organisms	Salmo gairdneri: 12.5 mg/l, 14 days: enzyme effect; change in enzyme activity 25.0 mg/l, 15 days: histological effect (presence of physical damage to tissues) (Petersen & Lech 1987) 50.0 mg/l, 7–15 days: histological effect: locomotor behaviour (quantifiable change in direct movement or activity) (Petersen et al. 1987).	
Other information	Manmade sources: in paper mill treated effluent: 0.47–1.2; 0.00047–0.0012 mg/l; colliery: coal washing effluent: 0.0018 mg/l; tailings lagoon: 0.039–0.042 mg/l; in sewage effluents: 0.280 mg/l (Verschueren 1983).	

38 • Acrylic acid

79-10-7

Synonyms	Propenoic acid Ethylenecarboxylic acid	
Sumformula of the chemical	CH2=CHCOOH	
Odour	Characteristic. Quality; rancid, sweet. Hedonic tone: unpleasant. Threshold Odour Concentration: absolute: 0.094 ppm 50% recognition: 1.04 ppm 100% recognition: 1.04 ppm. (Verschueren 1983). Quality: rancid, sweet Hedonic tone: unpleasant Threshold odour concentration: absolute: 0.094 ppm 50% recognition: 1.04 ppm 100% recognition: 1.04 ppm Odour index 100% recognition: 105 700 (Hellman & Small 1974).	
Molecular weight	72.06	
Specific gravity (water=1)	1.06	at 16 °C
Vapour density (air=1)	2.5	

Conversion factor, 1 ppm in air=	3 mg/m³
Conversion factor, 1 mg/m³ in air=	0.33 ppm
Vapour pressure, mmHg	3.2 at 20 °C 10 at 39 °C
Melting point, °C	12–14
Boiling point, °C	141
Log octanol/water coefficient, log Pow	0.31
Henry's law constant, Pa x m³/mol	0.04195 calc. (Yaws et al. 1991)
Total degradation in water	Biodegradation: 68% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	2500 orl-rat (Verschueren 1983)
LD50 values to birds in oral exposure, mg/kg	> 98 orl-Agelaius phoeniceus (Schafer et al. 1983)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida) 41 mg/l (Bringmann & Kühn 1980a)
LOEC values to algae, mg/l	0.15 rpd, act, Microcystis aeruginosa (Bringmann & Kuhn 1976) 18 rpd, act, Scenedesmus quadricauda (Bringmann & Kuhn 1980)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): algae (Microcystis aeruginosa): 0.15 mg/l green algae (Scenedesmus quadricauda): 18 mg/l Protozoa (Entosiphon sulcatum): 20 mg/l Protozoa (Uronema parduczi) 11 mg/l (Verschueren 1983).
Other information	Natural sources: produced by marine algae such as Phaeocystis and Polysiphonia lanosa; as a result of hydrolysis of dimethyl-β-propiothetin (Verschueren 1983).

39 • Acrylic acid, isobutyl ester 106-63-8

Synonyms	Isobutyl acrylate Propenoic acid, isobutyl ester
Odour	Quality: sweet, musty Hedonic tone: unpleasant to pleasant Threshold odour concentration absolute: 0.002 ppm 50% recognition: 0.009 ppm 100% recognition: 0.012 ppm Odour index 100% recognition: 525 000 (Hellman & Small 1974).
Log octanol/water coefficient, log Pow	2.22 (Sangster 1989)

LC50 values to fishes, mg/l	2.11	4d, Pimephales promelas (Geiger et al. 1988)

40 • Acrylonitrile

107-13-1

Synonyms	2-Propenenitrile Acrylon Cyanoethylene Vinylcyanide	
Sumformula of the chemical	CH2=CHCN	
Products containing the chemical	Acritet * 34% acrylonitrile + 60% CCl4 Ventox * = acritet Carbacryl * equal volumes of acrylonitrile and CCl4 Acrylofume * 3.95% acrylonitrile + 30% CCl4 + 30% chloroform* + 0.5% chloropicrin	
Use	Solvent. The major use of acrylonitrile is in the production of acrylic and modacrylic fibres by copolymerization with methylacrylate, methylmethacrylate, vinylacetate, vinylchloride, or vinylidenechloride. Other major uses include the manufacture of acrylonitrile-butadiene-styrene (ABS) and styrene-acrylonitrile (SAN) resins. Acrylonitrile is also used as a fumigant.	
State and appearance	Colourless liquid	
Odour	Characteristic. Quality: onion, garlic. Hedonic tone: pungent Threshold Odour Concentration: recognition: 3.72–51.0 mg/m³; 1.7–23 ppm; Population Identification Threshold (50%): 21.4 ppm Population Identification Threshold (100%): 21.4 ppm average: 18.6 ppm number of panellists: 16 41.9 mg/m³ = 19 ppm 45 mg/m³ = 20.4 ppm detection: 3.4 mg/m³ recognition: 47 mg/m³ (Verschueren 1983).	
Molecular weight	53.06	
Specific gravity (water=1)	0.8004	AT 25 °C
Vapour density (air=1)	1.83	
Conversion factor, 1 ppm in air=	2.203	mg/m³
Conversion factor, 1 mg/m³ in air=	0.454	ppm
Vapour pressure, mmHg	100 60	23 °C 11.8 °C (MITI 1992)
Water solubility, mg/l	73500 82000	20 °C (MITI 1992)
Melting point, °C	-83	(MITI 1992)
Boiling point, °C	77.3	(MITI 1992)
Log octanol/water coefficient, log Pow	0.3 0.25	(Yoshioka et al. 1986) (Sangster 1989)

A

Volatilization	Relative volatility (nBuAc=1) = 6.33
Photochemical degradation in air	Photo oxidation by ultraviolet light in aqueous medium at 50 °C: 24.2% degradation to CO2 after 24 hours (Verschueren 1983).
Photochemical degradation in water	Photo oxidation by ultra violet light in aqueous medium (50 °C): 24.2% degradation to CO2 after 24 hours (Verschueren 1983).
Total degradation in water	Biodegradation: 41–74% by BOD period: 14d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).
Other information about degradation	Biodegradation by mutant microorganisms (Verschueren 1983) - 500 mg/l at 20 °C disruption: mutant 100% in 4 hours Impact on biodegradation processes: BOD test is not influenced up to 1 g/l (Verschueren 1983). At 100 mg/l no inhibition of NH3 oxidation by Nitrosomonas sp (Verschueren 1983).
LD50 values to mammals in oral exposure, mg/kg	82 orl-rat (Lewis & Sweet 1984) 35 orl-mus (Verschueren 1983) 78 orl-rat (Verschueren 1983) 90 orl-gpg (Verschueren 1983)
LD50 values to mammals in non-oral exposure, mg/kg	148 skn-rat 250 skn-rbt (Lewis & Sweet 1984)
Other information about mammals	Rat inhalation: slight transitory effect: 129 ppm Rat inhalation: fatal: 636 ppm, 4 hours Rabbit inhalation: slight transitory effect: 97 ppm Rabbit inhalation: fatal: 258 ppm Cat inhalation: sometimes fatal: 152 ppm Guinea pig inhalation: slight transitory effect: 267 ppm Dog inhalation: very slight effects: 29 ppm Dog inhalation: 3/4: 110 ppm Rats: ingestion: 35 ppm (4 mg/kg body weight /day): mild signs of toxicity (decreased water and food consumption, decreased body weight). 100 ppm (10 mg/kg body weight /day) during 12 months: stomach papillomas (1 of 20 rats); central nervous system tumors (6 of 20 rats). Zymbal gland carcinoma (2 of 20 rats). Rats: inhalation: 80 ppm (6 hr/day, 5 days/week, 1 year): 3 of 26 rats; central nervous system tumors. (Verschueren 1983).
Effects on microorganisms	Pseudomonas putida: inhibition of cell multiplication starts at 53 mg/l (Verschueren 1983).
LC50 values to crustaceans, mg/l	6 96 hr, Crangon crangon (Adema 1976) 7.6 48 hr, Daphnia magna (LeBlanc 1980)

LC50 values to fishes, mg/l	11.6	96 hr, Lepomis macrochirus
	14.3	96 hr, Pimephales promelas
	33.5	96 hr, Poecilia reticulata (Jones 1971)
	32	48 hr, Oryzias latipes (Tonogai et al. 1982)
	25	96 hr, Branchydanio rerio
	13–28	48 hr, Leuciscus idus (Wellens 1982)
	24.5	24 hr, Lagodon rhomboides
	24	48 hr, Pimephales promelas
	14	96 hr, Gobius minutus, in sea water, 15 °C (Verschueren 1983)

41 • Actusol 53762-96-2

Use	Oil dispersant.	
LC50 values to fishes, mg/l	24	96 hr, Salmo gairdneri (Kemp et al. 1973)

42 • Adipic acid 124-04-9

Synonyms	Hexanedioic acid 1,4-Butanedicarboxylic acid
Sumformula of the chemical	COOH-(CH2)4-COOH
Molecular weight	146.14
Specific gravity (water=1)	1.37
Vapour density (air=1)	5.04
Water solubility, mg/l	15000 at 15 °C 23000 (MITI 1992)
Melting point, °C	150–153 (MITI 1992)
Boiling point, °C	265 100 mmHg (MITI 1992)
Log octanol/water coefficient, log Pow	0.08
Photochemical degradation in water	Photo oxidation by ultra violet light in aqueous medium at 90 –95 °C; time for the formation of CO2 (% of theoretical): 25%: 2.0 hr 50%: 5.0 hr 75%: 32.4 hr (Verschueren 1983).
Total degradation in water	Biodegradation: 68–90% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Other information about mammals	Mammals: rat: inhalation: no effect level: 126 g/l, 15 x 6 hr (Verschueren 1983).
Effects on microorganisms	Bacteria: no effect; 100 mg/l (Verschueren 1983).
LC50 values to fishes, mg/l	97 96 hr, Pimephales promelas (Vincent et al. 1976)

A

43 • Adiponitrile

111-69-3

Synonyms	1,4-Dicyanobutane Hexanedinitrile Adipic acid dinitrile Hexanedioic acid dinitrile Adipyldinitrile Tetramethylenedicyanide	
Sumformula of the chemical	CN-(CH2)4CN	
State and appearance	Colourless liquid.	
Molecular weight	108.15	
Specific gravity (water=1)	0.962 at 20/4 °C	
Vapour density (air=1)	3.73	
Conversion factor, 1 ppm in air=	4.5 mg/m^3	
Conversion factor, 1 mg/m^3 in air=	0.22 ppm	
Vapour pressure, mmHg	2 AT 119 °C	
Water solubility, mg/l	> 2000 (MITI 1992)	
Melting point, °C	0–1 (MITI 1992)	
Boiling point, °C	295–306 (MITI 1992)	
Total degradation in water	Biodegradation: 35–43% by BOD (NO2) (on the upward trend) period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	53–66% by BOD (NH3) (on the upward trend) period: 28d substance: 100 mg/l sludge: 30 mg/l
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987)	
LC50 values to fishes, mg/l	820 96 hr, Pimephales promelas 775 96 hr, Poecilia reticulata 720 96 hr, Lepomis macrochirus (Jones 1971)	

44 • Adogen 283 *

57157-80-9

Chemicals in the product	Aliphatic amines.
EC50 values to algae, mg/l	0.061 5d, rpd, Selenastrum capricornutum 0.027 5d, rpd, Asterionella formosa (Blanck 1984)
LC50 values to fishes, mg/l	1.3–9.7 120 hr, Salmo gairdneri (Dave et al. 1979)

45 • Adogen 383 *

35723-83-2

Chemicals in the product	Aliphatic amines.
EC50 values to algae, mg/l	0.555 5d, rpd, Monoraphidium 1.37 5d, rpd, Asterionella formosa (Blanck 1984)

46 • Aerozine-50 * 8065-75-6

Chemicals in the product	Hydrazine * 50%; Dimethylhydrazine * 50%	
Use	Rocket fuel.	
LC50 values to fishes, mg/l	2.25	96 hr, Lebistes reticulatus in hard water, 22–24.5 °C
	1.17	96 hr, Lebistes reticulatus in soft water, 22–24.5 °C (Verschueren 1983)

47 • Aflatoxin B1 1162-65-8

Effects on the physiology of water organisms	10 mg/kg, 2 days, cytogenetic effect (changes in the RNA and DNA of the cell): Ctenopharyngodon idella, Cyprinus carpio, Tinca tinca (Al-Sabti 1986).

48 • Alachlor 15972-60-8

Use	Herbicide.	
Molecular weight	270	
Log octanol/water coefficient, log Pow	3.22	(Anon. 1988)
Henry's law constant, Pa x m³/mol	0.0033	(Anon. 1988)
Mobility	Equilibrium distribution:	
		mass %
	air	0.09
	water	79.63
	solid	20.29
		(Anon. 1988).
Half-life in soil, days	18	(Li et al. 1990)
Effects on plants	Tubers of Cyperus rotundus L. were planted to soil sprayed with 0.25 kg alachlor/ha → a decrease in number of sprouts above ground (2 weeks after treatment) (Rincon & Warren 1979).	

49 • Alamine 336 * 68814-95-9

Chemicals in the product	* Alamine is a trademark for; a series of primary, secondary and tertiary aliphatic amines; organic substituted ammonia derivatives; * chain length from C12 to C18,; * with varying degrees of unsaturation	
Use	Corrosion inhibitors, ore flotation agents, textile finishing agents, rubber compounding (Verschueren 1983).	
EC50 values to algae, mg/l	0.08	5d, rpd, Selenastrum capricornutum (Blanck 1983)
LC50 values to fishes, mg/l	7.5–10	96 hr, Salmo gairdneri (Dave & Lindmann 1978)
	0.9–2.5	120 hr, Salmo gairdneri (Dave et al. 1979)

50 • Alanine

56-41-7

Synonyms	dl-Alanine dl-2-Aminopropanoic acid dl-α-Aminopropanoic acid
Sumformula of the chemical	CH3CH(NH2)COOH
Molecular weight	89.09
Water solubility, mg/l	166000 at 25 °C 322000 at 75 °C
Melting point, °C	295
Sublimation point, °C	200

51 • Aldicarb

116-06-3

Synonyms	2-Methyl-2(methylthio)propionaldehyde o-(Methylcarbomoyl)oxime Aldecarb Methylcarbamic acid o-((2-Methyl-2-(methylthio)propylidene)amino derivative Carbanolate 2-Methyl-2-(methylthio)propanal o-(Methylamino)carbonyl)oxime
Sumformula of the chemical	C7H14N2O2S
Products containing the chemical	Temik Temik 10G
Use	Soil applied insecticide, acaricide, and nematocide for use of cotton, sugar beets, potatoes, peanuts, ornamentals, yams, oranges, pecans, dry beans, soybeans, and sugarcane (Sax 1986).
State and appearance	White, crystalline solid. Soluble in water.
Odour	No odour (Sax 1986).
Molecular weight	190.29
Specific gravity (water=1)	1.195 at 25/20 °C
Vapour pressure, mmHg	0.0001 25 °C
Water solubility, mg/l	6000
Melting point, °C	99–101
Mobility	Leaching: leaching of aldicarb in Houston clay and Lufkin sandy loam is insignificant, but appeared to move more freely through columns of coarse sand (Verschueren 1983).
Hydrolysis in water	Aldicarb sulfoxide, the major metabolite of aldicarb, undergoes hydrolysis to form aldicarb oxime sulfoxide (Sax 1986).
Half-life in soil, days	7 in loam soil (Verschueren 1983) 70 (Li et al. 1990)

Total degradation in soil	Aldicarb degrades quite rapidly in soils with the evolution of CO2. Under field conditions a half-life of about 7 days in loam soil was found. The following metabolites were identified: aldicarbsulfoxide (2-methyl-2-(methylsulfinyl)propionalhyde-o- (methylcarbamoyl)-oxime and aldicarbsulfone (2-methyl-2-(methylsulfonyl)propionaldehyde-o-(methylcarbamoyl)-oxime (Verschueren 1983). Aldicarb penetrates deeply into soil. Sorption increases with increasing organic matter. – Aldicarb has a soil half-life of 1 to 2 weeks. Fungi cause the breakdown. The major degradation product is aldicarb sulfoxide but small quantities of the sulfone, oxime, nitrile sulfone, nitrile sulfoxide and oxime sulfoxide are also formed. Pure fungi cultures of Cunninghamella elegans, Gliocladium catenulatum, Penicillum multicolor, Trichoderma harzianum, and Rhyzoctonia sp. eventually degrade aldicarb to aldicarb amine sulfone and aldicarb alcohol sulfone. Aldicarb is toxic to springtails, collembola, mites and nematode, but is harmless to earthworms. – The degradation mechanism in soil is hydroxylation of the alkyl substituent or the aromatic moiety or by hydrolysis (Sax 1986).
Other information about degradation	Degrades quite rapidly in soils (Verschueren 1983). Residual protection against sucking and piercing pests lasts 10 weeks (Sax 1986).
Metabolism in plants	In plants, the sulfoxide is stable and persists up to 10 weeks. The sulfoxide either oxidizes to the sulfone or it undergoes hydrolysis to form the oxime sulfoxide. - Aldicarb uptake from the soil by plants is rapid. It is taken to the foliage (Sax 1986).
Other information about metabolism	Aldicarb is rapidly metabolized by animals by a combination of two pathways. The thioether may rapidly oxidize to the sulfoxide, then slowly oxidize to the sulfone. Or aldicarb may undergo hydrolysis or dealkylation to the oxime. Houseflies excrete 40% to 60% of a mixture of products after 24 hours. These products include aldicarb, the oxime, the oxime sulfoxide, the oxime sulfone, the sulfoxide, and the sulfone. – Detoxification in cattle takes place in the liver. The sulfone is the major product excreted (Sax 1986). Aldicarb was designed to resemble acetylcholine structurally and is a cholinesterase inhibitor. – Aldicarb sulfoxide is 76 times more powerful as a cholinesterase inhibitor than is aldicarb. – Aldicarb at 5 ppm inhibits Azotobacter chroococcum beij growth by altering its glucose metabolism (Sax 1986).
LD50 values to mammals in oral exposure, mg/kg	0.6 orl-rat (Lewis & Sweet 1984) 0.9 orl-rat, technical aldicarb (Verschueren 1983) 0.3 orl-mus (Sax 1986)
LD50 values to mammals in non-oral exposure, mg/kg	2.5 skn-rat 1400 skn-rbt (Lewis & Sweet 1984) > 5.0 skn-rbt, technical aldicarb (Verschueren 1983) 2400 skn-gpg (Sax 1986)
Other information about mammals	ALD = 1.6 mg/kg, act, orl, deer mouse LDfr = 55.2 mg/kg, subacute, deer mouse (Virtanen & Nuuja 1987).
Health effects	Symptoms of cholinesterase inhibition include pupillary constriction, anorexia, nausea, vomiting, diarrhea, salivation, muscle twitching, convulsions, bronchoconstriction, and respiratory failure (Sax 1986).
Carcinogenicity	NCI carcinogenesis bioassay completed: results negative; mus, rat (Lewis & Sweet 1984)
Mutagenicity	Mutagen data: otr, rat, emb, 0.117 mg/plate (Sax 1986).

LD50 values to birds in oral exposure, mg/kg	3.4 4.44 1.78 4.22 4.22 0.75 0.75 3.16	orl-dck (Lewis & Sweet 1984) orl-dck (Sax 1986) orl-Agelaius phoeniceus orl-Sturnus vulgaris orl-Coturnix coturnix orl-Passer domesticus orl-Quiscalus quiscula orl-Columba livia (Schafer et al. 1983)
EC50 values to microorganism, mg/l	2150	INT (Dutton et al. 1986)
LC50 values to crustaceans, mg/l	0.012 0.016 0.209 0.07	96 hr, Penaeus duorarum 96 hr, Mysidopsis bahia (Anon.1981) 48 hr, Daphnia laevis 48 hr, D.laevis, juvenile (Foran et al. 1985)
EC50 values to crustaceans, mg/l	0.051 0.065	48 hr, mbt, Daphnia laevis 48 hr, mbt, D.laevis, juvenile (Foran et al. 1985)
LC50 values to fishes, mg/l	8.8 0.041 0.08	96 hr, Salmo gairdneri 96 hr, Cyprinodon variegetus 96 hr, Lagodon rhomboides (Anon.1981)
LOEC values to fishes, mg/l	0.16	srv, schr, Pimephales promelas (Pickering & Gilliam 1982)
NOEC values to fishes, mg/l	0.078	srv, schr, Pimephales promelas (Pickering & Gilliam 1982)
Effects on the physiology of water organisms	Barbus conchonius, 15 d, 0.484 mg/l, hematological effect (Pant et al. 1987).	
Other information about water organisms	8.8 mg/l, 96 hr, orl, Salmo gairdneri, LD50 (Sax 1986).	

52 • Aldrin

309-00-2

Synonyms	1,2,3,4,10,10-Hexachloro-1,4,4a,5,8,8a-hexahydro-1,4-endo, exo-5,8-dimethanonaphthalene	
Products containing the chemical	Compound 118 Octalene	
Use	Insecticide; fumigant.	
State and appearance	Brown and white crystalline solid	
Odour	Odour threshold: 0.017 mg/kg water (Verschueren 1983).	
Molecular weight	364.9	
Vapour pressure, mmHg	0.000023 20 °C	
Water solubility, mg/l	< 0.1	(MITI 1992)
Melting point, °C	104–105.5	(MITI 1992)
Log octanol/water coefficient, log Pow	5.52–7.40 6.23 6.75	(Sabljic 1987) Anon. 1988 (MITI 1992)
Henry's law constant, Pa x m³/mol	280	(Anon. 1988)

Mobility	Equilibrium distribution: *mass %* air 27.07 water 0.28 solid 72.65 (Anon. 1988).
Photochemical degradation in air	Photochemical transformations (Verschueren 1983): Aldrin → Dieldrin ↓ ↓ Photoaldrin → Protodieldrin
Photochemical degradation in water	Photo oxidation by ultra violet light in aqueous medium at 90–95 °C time for the formation of CO2 (% of theoretical): 25%: 14.1 hr 50%: 28.2 hr 75%: 109.7 hr((Verschueren 1983)).
Half-life in water, days	7.7 calculated halftime in water at 25 °C and 1 m depth, based on evaporation rate of 0.00372 m/hr (Verschueren 1983)
Total degradation in soil	Disappearance from soils: 75–100% in 1–6 years (Verschueren 1983).
Total degradation in water	Conversion of aldrin to dieldrin was 80% complete after 8 weeks in river water kept in a sealed jar under sunlight and artificial fluorescent light (initial concentration 10 µg/l) (Verschueren 1983). Persistence in river water in a sealed glass jar under sunlight and artificial fluorescent light (initial conc. 10 µg/l): *% of original compound found* after: 1 hr 100; 1 week 100; 2 week 80; 4 week 40; 8 week 20 (Verschueren 1983). Biodegradation: 0% by BOD period: 17.5 d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Other information about metabolism	Metabolic pathway of aldrin and dieldrin under oceanic conditions (Verschueren 1983): Aldrin Dieldrin Photodieldrin I I I V V V Aldrin diol
Bioconcentration factor, fishes	3490–20000 10w, Cyprinus carpio, conc 0.001 mg/l 1550–9450 10w, Cyprinus carpio, conc 0.0001 mg/l (Lipid 7.0%) 1040–5980 10w, Cyprinus carpio, conc 0.001 mg/l 735–4860 10w, Cyprinus carpio, conc 0.0001 mg/l (Lipid 1.7%) (MITI 1992)
Bioconcentration factor, mollusca	350–4500 (Verschueren 1983)

A

Other information about bioaccumulation	Confirmed to be accumulated on a high level (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	39 orl-rat 50 orl-rbt (Lewis & Sweet 1984) 67 orl-rat (Verschueren 1983)
LD50 values to mammals in non-oral exposure, mg/kg	98 skn-rat (Lewis & Sweet 1984) 39–60 ukn-rat (Virtanen & Nuuja 1987) 98–200 skn-rat (Verschueren 1983)
LDLo values to mammals in non-oral exposure, mg/kg	15 skn-rbt (Lewis & Sweet 1984)
Other information about mammals	Ingestion: rats fed for two years at dietary level of 5 ppm suffered no ill effects but liver damage resulted at the 25 ppm level (Verschueren 1983).
Carcinogenicity	NCI carcinogenesis bioassay completed: results positive, mus; negative, rat (Lewis & Sweet 1984).
LD50 values to birds in oral exposure, mg/kg	7 orl-bwd 10 orl-ckn (Lewis & Sweet 1984) 23.7 orl-Agelaius phoeniceus 5.00–23.7 orl-Sturnus vulgaris 42.2 orl-Coturnix coturnix 13.3 orl-Passer domesticus 7.5 orl-Quiscalus quiscula 56.2 orl-Columba livia (Schafer et al. 1983)
Other information about birds	Quail: acceptable LD50: 4 mg/kg (Verschueren 1983). FAO/WHO Residue tolerance limit: 0.03–0.3 mg/kg/day (Verschueren 1983).
Effects on arthropods	LC50 Acroneuria pacifica: 96 hr, 0.200 mg/l (Verschueren 1983) LC50 Pteronarcys californica: 30 d, 0.0025 mg/l (Jensen & Gaufin 1966) LC50 Pteronarcys californica: 96 hr, 0.0013 mg/l (Verschueren 1983) LC50 Pteronarcys californica: 96 hr, 0.180 mg/l (Verschueren 1983) LC50 Aades aegypti: 24 hr, 0.003 mg/l (Khan et al. 1973) LC50 Chironomus riparius: 24 hr, 0.0008 mg/l (Estenik & Collins 1979) LC50 Ranatra elongata: 96 hr, 0.043 mg/l (Shukla et al. 1982) LD50, house fly, Musca, 3 days old, female: 0.014 mg/fly (Verschueren 1983). Hydropsyche larvae: significant modification of net construction after 48 hours exposure: 0.020 mg/l (Verschueren 1983).

LC50 values to crustaceans, mg/l	0.028	48 hr, Daphnia magna (Sanders & Cope 1966)
	0.03	act, D.pulex (Frear et al. 1967)
	0.008	96 hr, Crangon septemspinosa
	0.009	96 hr, Palaemonetes vulgaris (Eisler 1969)
	8	96 hr, Asellus brevicaudus
	28	96 hr, Daphnia pulex
	23	96 hr, Simocephalus serrulatus (Sanders 1970)
	0.27	48 hr, D.magna (Gorbach & Knauf 1971)
	0.029	act, D.magna (Kenaga 1979)
	50	96 hr, Palaemonetes kadiakensis
	0.00074	96 hr, Palaemonon macrodactylus
	9800	96 hr, Gammarus lacustris
	0.08	24 hr, Asellus
	4300	96 hr, Gammarus fasciatus (Verschueren 1983)
	0.023	1d, Macrobrachium lamarrei
	0.005	2d, Macrobrachium lamarrei
	0.0023	3d, Macrobrachium lamarrei (Mary et al. 1986)
EC50 values to crustaceans, mg/l	0.028	48 hr, Daphnia pulex (Shapiro 1979)
LC50 values to fishes, mg/l	0.028	96 hr, Pimephales promelas
	0.013	96 hr, Lepomis macrochirus (Henderson et al. 1959)
	0.018	96 hr, Salmo gairdneri
	0.046	96 hr, Oncorhynchus kisutch
	0.0075	96 hr, Oncorhynchus tshawytscha (Katz 1961)
	0.004	96 hr, Fundulus heteroclitus (Eisler 1970b)
	0.02	96 hr, Poecilia reticulata (Macek & McAllister 1970)
	0.036	96 hr, Salmo gairdneri (Edwards 1977)
	0.002	Salmo gairdneri
	0.005	Lepomis macrochirus
	0.008	Pimephales promelas (Kenaga 1979)
	0.175	96 hr, Heteropneustes fossilis (Srivastava & Singh 1981)
	0.004	96 hr, Cyprinus carpio (Verschueren 1983)
	0.017	96 hr, Poecilia reticulata (Gupta et al. 1984)
	0.008	96 hr, Fundulus heteroclitus
	0.017	96 hr, Fundulus majalis
	0.021	96 hr, Fundulus diaphanus
	0.013	96 hr, Menidia menidia
	0.1	96 hr, Mugil cephalus

	0.012 96 hr, Thalassoma bifasciatum 0.036 96 hr, Sphaeroides maculatus 0.016 96 hr, Anguilla rostrata 0.005 96 hr, Anguilla rostrata 0.042 96 hr, Roccus americanus 0.02 96 hr, Lepomis gibbosus 0.01 96 hr, Salmo gairdneri 0.01 96 hr, Morone saxatilis (Verschueren 1983) 0.175 96 hr, Heteropneustes fossilis (Srivastava & Srivastava 1988) 0.075 48 hr, Oryzias latipes (MITI 1992)
Effects on the physiology of water organisms	Barbus conchonius, 60–120 d, 0.0000466 mg/l, histological effect (Kumar & Pant 1988). Heteropneustes fossilis, 4 d, 0.140 mg/l, hematological effect (Srivastava & Srivastava 1988). Tilapia mossambica, 3–20 d, 0.010 mg/l, physiological effect (Mohamed et al. 1987). Tilapia mossambica, 30 d, 0.100 mg/l, hematological effect (Ghosh & Chatterjee 1987).
Other information about water organisms	Hard clam (Mercennaria mercennaria): 10 day two-cell stage fertilized, 500 ppb, 37% survival; 10 day eggs introduced into test media, 1000 ppb, 0% survival (Verschueren 1983).

53 • Aliquat 336 * 5137-55-3

Chemicals in the product	Aliphatic amines
EC50 values to algae, mg/l	0.169 5d, rpd, Selenastrum capricornutum 0.018 5d, rpd, Monoraphidium 0.025 5d, rpd, Asterionella formosa (Blanck 1984)
LC50 values to fishes, mg/l	0.094–0.137 96 hr, Branchydanio rerio (Dave et al. 1981) 0.5–0.87 120 hr, Salmo gairdneri (Dave et al. 1979)

54 • Alkyl(C=8-11)diphenyl phosphate 29761-21-5

Sumformula of the chemical	C22H3104P
Water solubility, mg/l	< 10 (MITI 1992)
Melting point, °C	< -30 (MITI 1992)
Total degradation in water	Biodegradation: 0–1% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	168–363 8w, Cyprinus carpio, conc 0.1 mg/l 223–1120 8w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
LC50 values to fishes, mg/l	11.7 48 hr, Oryzias latipes (MITI 1992)

55 • Alkyl dimethylbenzyl ammonium chloride

8001-54-5

Synonyms	Benzalkonium chloride Alkyl(C=10-14)(benzyl)dimethylammoniumchloride	
Use	Microbicide.	
Water solubility, mg/l	> 1000 (C=10-14) (MITI 1992)	
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l C=10-14 (MITI 1992).	
Bioconcentration factor, fishes	< 0.2–5.9	6w, Cyprinus carpio, conc 0.5 mg/l
	< 1.8–8.6	6w, Cyprinus carpio, conc 0.05 mg/l, C=10-14 (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987) *(alkyl (C10~14) (benzyl) dimethyl ammonium chloride).	
LC50 values to fish, mg/l	0.62	96 hr, Rasbora heteromorpha
	1.1	48 hr, Rasbora heteromorpha (Tooby et al. 1975)
	9.21	48 hr, Oryzias latipes (C=10-14) (MITI 1992)

56 • Alkylethoxylate

LC50 values to fishes, mg/l	1.2–1.4	96 hr, Pimephales promelas (Maki et al. 1979)
LOEC values to fishes, mg/l	0.2	srv, chr, Pimephales promelas (Maki 1979)
NOEC values to fishes, mg/l	0.18	srv, chr, Pimephales promelas (Maki 1979)

57 • Alkylethoxysulfate

LC50 values to fishes, mg/l		* chain length C12-15:
	1.0–2.5	96 hr, Salmo trutta (Reiff et al. 1979)
	3.3–6.2	96 hr, Leuciscus idus (Reiff et al. 1979)
	5.7	48 hr, Carassius auratus (Reiff et al. 1979)
	3.9	48 hr, Rasbora heteromorpha (Reiff et al. 1979)
LOEC values to fishes, mg/l	0.22	srv, grw, chr, Pimephales promelas (Maki 1979)
NOEC values to fishes, mg/l	0.1	srv, grw, chr, Pimephales promelas (Maki 1979)

58 • Alkylsulfate

EC50 values to algae, mg/l	60	grw, 48 hr, Selenastrum capricornutum (Atsuko et al. 1984)

59 • Allethrin 584-79-2

Synonyms	d-trans-Allethrin 3-Allyl-2-methyl-4-oxocyclopenthe-2-enyl-2,2-dimethyl-3-(2- methyl-prop-1-enyl)-cyclopropylcarboxylate dl-2-Allyl-4-hydroxy-3-methyl-2-cyclo–penten-1-one ester of d-trans-chrysanthemum monocarboxylic acid Allylhomologue of cinerin I	
Chemicals in the product	* a mixture of; cis and trans allethrins	
Use	Synthetic insecticide.	
State and appearance	Clear, amber-coloured, viscous liquid.	
Molecular weight	302.45	
Specific gravity (water=1)	1.01	at 20/20 °C
Boiling point, °C	160	
LD50 values to mammals in oral exposure, mg/kg	425	orl-rat (Lewis & Sweet 1984)
	860	d-trans-, orl-rat (Pesticide Dictionary 1976)
	480	orl-mus (Martin 1968)
Effects on arthropods	LC50, 96 hr, 0.0021 mg/l, Pteronarcys californica (Sanders & Cope 1968).	
	Fourth instar larval Chironomus riparius: LC50, 24 hr, 41.9 ppb (Estenik & Collins 1979).	
LC50 values to crustaceans, mg/l	0.056 0.021	48 hr, Simocephalus serrulatus 48 hr, Daphnia pulex (Sanders & Cope 1966)
	0.011	96 hr, Gammarus lacustris (Sanders 1969)
	0.008	96 hr, Gammarus fasciatus (Sanders 1972)
	0.21	act, Daphnia pulex (Kenaga 1979)
LC50 values to fishes, mg/l	0.0096 0.0097 0.0099	96 hr, Oncorhynchus kisutch 96 hr, Salmo gairdneri 96 hr, Perca flavescens (Mauck & Olson 1976)
	0.019	act, Salmo gairdneri (Kenaga 1979)
	30.1	act, Ictalurus punctatus (Pesticide Manual 1983)
	0.019 0.056	96 hr, Salmo gairdneri 96 hr, Lepomis macrochirus (Verschueren 1983)
LOEC values to fishes, mg/l	0.0165	srv, 48 hr, Salmo salar (Zitko et al. 1977)
Other information about water organisms	LC50 Pteronarcys californica: 96 hr,0.0021 mg/l (Sanders & Cope 1968)	

60 • Allyl isothiocyanate 57-06-7

Synonyms	Mustard oil 2-Propenyl isothiocyanate Allylisosulfo-cyanate
Sumformula of the chemical	CH2=CHCH2NCS
Use	Fumigant; ointments and mustard plasters; military poison gas.
Odour	Characteristic: mustard oil; irritant.

Molecular weight	99.15	
Specific gravity (water=1)	1.015	at 15/4 °C
Vapour density (air=1)	3.4	
Conversion factor, 1 ppm in air=	4.12	mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.243	ppm
Vapour pressure, mmHg	1 10	at -2 °C at 38.3 °C
Water solubility, mg/l	2000	
Melting point, °C	-100	
Boiling point, °C	151	
Log octanol/water coefficient, log Pow	2.11	
Other information about degradation	Impact on biodegradation processed: 75% inhibition of the nitrification process in activated sludge at 1.9 mg/l (Verschueren 1983).	

61 • Allyl phenyl ether

1746-13-0

Sumformula of the chemical	C9H10O	
Log octanol/water coefficient, log Pow	2.9 2.94	(Anon. 1986) (Sangster 1989)

62 • 4-Allyl-1,2-dimethoxybenzene

93-15-2

Synonyms	2-Methoxy-4-propenylphenolmethylether	
Water solubility, mg/l	500	(MITI 1992)
Boiling point, °C	249	(MITI 1992)
Total degradation in water	Biodegradation: 86–91% by BOD period: 28w substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LD50 values to birds in oral exposure, mg/kg	> 316 > 316	orl-Agelaius phoeniceus orl-Sturnus vulgaris (Schafer et al. 1983)

63 • Allylacetate

591-87-7

Synonyms	2-Propenylethanoate
Sumformula of the chemical	CH3COOCH2CH=CH2
Molecular weight	100.11
Specific gravity (water=1)	0.928

Conversion factor, 1 ppm in air=	4.1	mg/m³
Conversion factor, 1 mg/m³ in air=	0.245	ppm
Boiling point, °C	103–104	
LD50 values to mammals in oral exposure, mg/kg	130	orl-rat (Patty 1967)

64 • Allylalcohol

107-18-6

Synonyms	Propenylalcohol 2-Propen-1-ol Propenol-3 Vinylcarbinol	
Sumformula of the chemical	CH2=CH-CH2OH	
Use	Contact pesticide for weed seeds and certain fungi; solvent.	
Odour	Characteristic. Quality: alcoholic. Hedonic tone: not unpleasant. (Verschueren 1983) Faint odour: 0.017 mg/l water (Verschueren 1983).	
Molecular weight	58.09	
Specific gravity (water=1)	0.825	at 20/4 °C
Vapour density (air=1)	2	
Conversion factor, 1 ppm in air=	2.414	mg/m³
Conversion factor, 1 mg/m³ in air=	0.414	ppm
Vapour pressure, mmHg	20 32	20 °C 30 °C
Melting point, °C	-129	(MITI 1992)
Boiling point, °C	96.9	(MITI 1992)
Log octanol/water coefficient, log Pow	0.17	(Sangster 1989)
Henry's law constant, Pa x m³/mol	0.5638	calc. (Yaws et al. 1991)
Volatilization	Relative volatility (nBuAc=1) = 1.47	
Photochemical degradation in water	Photo oxidation by ultra violet light in aqueous medium at 50 °C: 13.9% degradation of CO2 after 24 hours (Knoevenagel & Himmelreich 1976).	
Chemical oxygen demand, g O2/g	2.12	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g O2/g	1.79	5 days (Bridie et al. 1979)

Total degradation in water	Biodegradation: 86% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
Other information about degradation	Impact on biodegradation processes: 75% inhibition of the nitrification process in activated sludge at 19.5 mg/l (Verschueren 1983).	
LD50 values to mammals in oral axposure, mg/kg	64 96 71 64–105	orl-rat (Lewis & Sweet 1984) orl-mus orl-rbt orl-rat (Patty 1967)
LD50 values to mammals in non-oral exposure, mg/kg	45	skn-rbt (Lewis & Sweet 1984)
LC50 values to mammals in inhalation exposure, mg/m^3	500	2 hr, ihl-mus (Lewis & Sweet 1984)
LC50 values to mammals in inhalation exposure, ppm	165 76	4 hr, ihl-rat (Lewis & Sweet 1984) 8 hr, ihl-rat (Patty 1967)
LDLo values to mammals in oral exposure, mg/kg	5	orl-rat (Lewis & Sweet 1984)
Other information about mammals	Rat: repeated ingestion no effect 4–12 mg/kg Rat: inhalation no effect 20 ppm, 60 x 7 hr (Patty 1967).	
Health effects	Man: slight eye irritation: 6.25 ppm nasal irritation: < 0.78 ppm pulmonary discomfort: > 25 ppm (Patty 1967).	
Effects on plants	Highly phytocidal (Martin 1968).	
LC50 values to fishes, mg/l	1	24 hr, Carassius auratus (Bridie et al. 1979)
Other information about water organisms	LC50 Mercennaria mercennaria: 12 d, 0.25 mg/l 48 hr, 1.0 mg/l (Kemp et al.1973)	

65 • Allylamine

107-11-9

Synonyms	2-Propenylamine	
Sumformula of the chemical	CH2=CHCH2NH2	
Odour	Characteristic: similar to ammonia, irritating. Threshold Odour Concentration: 6.3 ppm; < 6 mg/m^3; 14 mg/m^3 Faint odour: 0.067 mg/l water. (Verschueren 1983).	
Molecular weight	57.07	
Specific gravity (water=1)	0.76	at 20/4 °C
Vapour density (air=1)	2	
Conversion factor, 1 ppm in air=	2.33	mg/m^3

Conversion factor, 1 mg/m³ in air=	0.428 ppm
Boiling point, °C	53
Other information about degradation	Degradation by Aerobacter (200 mg/l, 30°): parent 78% in 93 hr; mutant 100% in 13 hr (Verschueren 1983).
LD50 values to mammals in oral exposure, mg/kg	106 orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	35 skn-rbt (Lewis & Sweet 1984)
LC50 values to mammals in inhalation exposure, ppm	286 ihl-rat 177 ihl-rat (Patty 1967)
Other information about mammals	Rat: inhalation: deaths 40 ppm, 50 x 7 hr Rat: inhalation: reduced growth: 5 ppm, 50 x 7 hr (Patty 1967).
Effects on amphibia	Mexican axoloth (3–4 weeks after hatching): 48 hr LC50: 1.8 mg/l Clawed toad (3–4 weeks after hatching): 48 hr LC50: 5.0 mg/l (Slooff & Baerselman 1980).
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): Bacteria (Pseudomonas putida): 700 mg/l (Bringmann & Kühn 1980).
LOEC values to algae, mg/l	0.35 Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to crustaceans, mg/l	28 48 hr, Daphnia cucullata (Canton & Adema 1978) 100 48 hr, Asellus aquaticus (Slooff 1983) 130 48 hr, Gammarus pulex (Slooff 1983)
LC50 values to fishes, mg/l	15 48 hr, Salmo gairdneri (Slooff et al. 1983)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): Algae (Microcystis aeruginosa: 0.35 mg/l Green algae (Scenedesmus quadricauda); 2.2 mg/l Protozoa (Entosiphon sulcatum: 23 mg/l Protozoa (Uronema parduczi): 3140 mg/l (Bringmann & Kühn 1976, 1980a, 1980b). LC50, 48 hr, 18 mg/l, Tubificidae LC50, 48 hr, 14 mg/l, Chironomus gr. thummi LC50, 48 hr, 26 mg/l, Erpobdella octoculata LC50, 48 hr, 5 mg/l, Lymnaea stagnalis LC50, 48 hr, 66 mg/l, Dugesia cf. lugubris LC50, 48 hr, 17.5 mg/l, Hydra oligactis LC50, 48 hr, 120 mg/l, Corixa punctata LC50, 48 hr, > 180 mg/l, Ischura elegans LC50, 48 hr, 100 mg/l, Nemoura cinerea LC50, 48 hr, 30 mg/l, Cloeon dipterum (Slooff 1983)

66 • Allylbromide 106-95-6

Synonyms	3-Bromopropene
Sumformula of the chemical	C3H5Br
Log octanol/water coefficient, log Pow	1.79 (Sangster 1989)

Chemical oxygen demand, g 02/g	0.72	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.59	5 days (Bridie et al. 1979)
LC50 values to fishes, mg/l	0.8	24 hr, Carassius auratus (Bridie et al. 1979)

67 • Allylchloride

107-05-1

Synonyms	3-Chloro-1-propene Chloroallylene 3-Chloro-1-propylene	
Sumformula of the chemical	CH2=CH-CH2Cl	
State and appearance	Colourless to pale yellow.	
Odour	Characteristic: garlic-onion pungency, green. Threshold Odour Concentration; 0.660 mg/m³ = 0.21 ppm 50% recognition: 0.21 ppm 100% recognition: 25 ppm Population Identification Threshold 50: 0.21 ppm Population Identification Threshold 100: 0.47 ppm (Verschueren 1983).	
Molecular weight	76.53	
Specific gravity (water=1)	0.94	at 20/4 °C
Vapour density (air=1)	2.64	
Conversion factor, 1 ppm in air=	3.18	mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.314	ppm
Vapour pressure, mmHg	340 440	20 °C 30 °C
Water solubility, mg/l	2300	(MITI 1992)
Melting point, °C	-134.5	(MITI 1992)
Boiling point, °C	45	(MITI 1992)
Henry's law constant, Pa x m^3/mol	919.2	calc. (Yaws et al. 1991)
Chemical oxygen demand, g 02/g	0.86	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.23	5 days (Bridie et al. 1979)
Total degradation in water	Biodegradation: 55–69% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
Other information about degradation	Impact on biodegradation processes: 75% decrease of nitrification by activated sludge at 180 mg/l (Meinck et al. 1970).	

Bioconcentration factor, fishes	< 0.14–0.88 < 1.3–5.60	6w, Cyprinus carpio, conc 0.5 mg/l 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
LD50 values to mammals in oral exposure, mg/kg	64 700	orl-rat (Lewis & Sweet 1984) orl-rat (Patty 1967)
LD50 values to mammals in non-oral exposure, mg/kg	2066	kn-rbt (Lewis & Sweet 1984)
Other information about mammals	Rat: max, exposure time concentrations: 290 ppm, 3 hr inhalation: 2900 ppm, 1 hr 29300 ppm, 15 min Rat, guinea pig, rabbit: liver injury: 8 ppm, 7 hr/day, 5 days/w, 28 days Rat, guinea pig, rabbit: died after 127–134 exposures at 3 ppm (Patty 1967).	
Health effects	Man: very irritating to the eyes and upper respiratory tract eye irritating 50–100 ppm (Patty 1967)	
Carcinogenicity	NCI carcinogenesis bioassay completed: results indefinite, mus; negative, rat (Lewis & Sweet 1984).	
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 115 mg/l (Bringmann & Kühn 1980a).	
LOEC values to algae, mg/l	6.3	Scenedesmus quadricauda (Bringmann & Kühn 1980a)
LC50 values to fishes, mg/l	19.8 10 1.2 6.9	96 hr, Pimephales promelas (Pickering & Henderson 1966) 24 hr, Carassius auratus (Bridie et al. 1979) 14 d, Poecilia reticulata (Hermens et al. 1985) 48 hr, Oryzias latipes (MITI 1992)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda: 6.3 mg/l protozoa (Entosiphon sulcatum): 8.4 mg/l protozoa (Uronema parduczi): > 240 mg/l (Bringmann & Kühn 1980a, 1980b).	
Other information	Hardness of water decreases toxicity (Pickering & Henderson 1966).	

68 • Allylcyanide 109-75-1

Synonyms	3-Butenenitrile Allylnitrile	
Sumformula of the chemical	C4H5N	
Log octanol/water coefficient, log Pow	0.4	(Sangster 1989)
LC50 values to fishes, mg/l	182	96 hr, Pimephales promelas (Broderius & Kahl 1985)

69 • Allylglycidylether 106-92-3

Synonyms	2-Propenyloxy-2,3-epoxypropane AGE Allyl 2,3-epoxypropylether 1-Allyloxy-2,3-epoxypropane 1,2-Epoxy-3-allyloxypropane Glycidylallylether ((2-Propenyloxy)methyl)oxirane

Use	Component of epoxy resin systems. The epoxy group of the glycidylether reacts during the curing process and glycidylethers are therefore generally no longer present in completely cured products.	
State and appearance	Colourless liquid.	
Odour	Threshold value: 47 mg/m³ (Verschueren 1983).	
Molecular weight	114.15	
Specific gravity (water=1)	0.969	at 20/4 °C
Vapour density (air=1)	3.94	
Conversion factor, 1 ppm in air=	4.74	mg/m³
Conversion factor, 1 mg/m³ in air=	0.21	ppm
Vapour pressure, mmHg	3.6 5.8	at 20 °C at 30 °C
Water solubility, mg/l	141000	
Boiling point, °C	153.9	
Solidification point, °C	-100	forms glass
Chemical oxygen demand, g O2/g	1.99	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g O2/g	0.06	5 days (Bridie et al. 1979)
LD50 values to mammals in oral exposure, mg/kg	390 1600	orl-mus orl-rat (Patty 1967)
LC50 values to mammals in inhalation exposure, ppm	270 670	4 hr, ihl-mus 8 hr, ihl-rat (Patty 1967)
Other information about mammals	Rat: 400 mg/kg i.m. injections on days 1, 2, 8 and 9; animals sacrified on day 12; focal necrosis of the testis in 1 of 2 of the 3 surviving rats, atrophy of loss of lymphoid tissue in 2 of 3 rats, decreased leukocyte count (Kodama et al. 1961).	
LC50 values to fishes, mg/l	30 78	96 hr, Carassius auratus 24 hr (Bridie et al. 1979)

70 • Allylidene diacetate

869-29-4

Sumformula of the chemical	C7H10O4	
Water solubility, mg/l	9900	(MITI 1992)
Boiling point, °C	184	(MITI 1992)
Log octanol/water coefficient, log Pow	0.78	(MITI 1992)
Total degradation in water	Biodegradation: 78–82% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

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71 • Allyloxycarb 6392-46-7

Other information about mammals	ALD = 62.0 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987).
LD50 values to birds in oral exposure, mg/kg	13.3 orl-Agelaius phoeniceus 10.0–13.3 orl-Sturnus vulgaris (Schafer et al. 1983)

72 • 2-Allylphenol 1745-81-9

LC50 values to fishes, mg/l	13.2 96 hr, Pimephales promelas (Holcombe et al. 1984)

73 • Allylthiourea 109-57-9

Synonyms	Allylsulfocarbamide Thiosinamine Allylsulfourea
Sumformula of the chemical	C3H5NHCSNH2
Use	Medicine; corrosion inhibitor, organic synthesis.
State and appearance	White crystalline solid.
Odour	Slight garlic odour; bitter taste.
Specific gravity (water=1)	1.22
Melting point, °C	78
Other information about degradation	Impact on biodegradation processes: approximately 50% inhibition of NH3 oxidation by Nitrosomonas at 1.2 mg/l (Hooper & Terry 1973).
Other information about mammals	LDfr = 100 mg/kg/day, subacute, deer mouse (5-allyl-thiourea) (Virtanen & Nuuja 1987).
Effects on microorganisms	Toxicity threshold (cell multiplication test): bacteria (Pseudomonas putida): 140 mg/l (Bringmann & Kühn 1980a).
LOEC values to algae, mg/l	41 rpd, act, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
Other information about water organisms	Toxicity threshold (cell multiplication test): green algae (Scenedesmus quadricauda: 41 mg/l protozoa (Entosiphon sulcatum): 13 mg/l (Bringmann & Kühn 1980a).

74 • Allyltriphenyltin 76-63-1

Other information about mammals	LDfr = 68.8 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

75 • Aluminium and aluminium compounds 7429-90-5

Molecular weight	26.98
LD50 values to birds in oral exposure, mg/kg	> 111 orl-Agelaius phoeniceus > 250 orl-Passer domesticus (Schafer et al. 1983)

Effects on plants	> 0.5 ppm (0.01 meq/100 g) Al in the soil injure cotton and alfalfa (Foy 1974).	
LC50 values to crustaceans, mg/l	6.57 4.37	48 hr, mbt, Asellus aquaticus, Al(III) 96 hr, mbt, Asellus aquaticus, Al(III) (Martin & Holdich 1986)
	1.4 3.9	21d, Daphnia magna 48 hr, without food, D.magna (Biesinger & Christensen 1972)
EC50 values to crustaceans, mg/l	0.68	21d, rpd, Daphnia magna (Biesinger & Christensen 1972)
LOEC values to crustaceans, mg/l	0.32	21d, rpd, Daphnia magna (Biesinger & Christensen 1972)
LC50 values to fishes, mg/l	0.56	28d, Salmo gairdneri (Birge et al. 1980)
LOEC values to fishes, mg/l	0.1 0.2 0.1	srv, act, Catostomus commersoni srv, act, Salvelinus fontinalis Stizostedium vitreum pH 4.2–5.6 (Baker & Schofield 1982)

76 • Aluminium chloride 7446-70-0

LC50 values to crustaceans, mg/l	3.9	48 hr, Daphnia magna (Biesinger & Christensen 1972)

77 • Aluminium sulfate 10043-01-3

Synonyms	Aluminium trisulfate Sulfuric acid, aluminum salt	
Sumformula of the chemical	012S3.2Al	
Molecular weight	342.14	
LD50 values to mammals in oral exposure, mg/kg	6207	orl-mus (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	1735	ipr-mus (Sweet 1987)
TDLo values to mammals in non-oral exposure, mg/kg	27.371 27.371	intratesticulat-rat, paternal eff. scu-mus, paternal effects (Sweet 1987)
EC50 values to crustaceans, mg/l	6.57 4.37 12.8 9.19	mbt, 2d, Asellus aquaticus mbt, 3d, Asellus aquaticus mbt, 2d, Crangonyx pseudogracilis mbt, 4d, Crangonyx pseudogracilis (Martin & Holdich 1986)
Effects on the physiology of water organisms	Micropterus dolomieui, 30 d, 0.2516 mg/l, growth effect; 4–30 d, 0.032–0.2516 mg/l mortality (Kane & Rabeni 1987). Salmo gairdneri, 4 d, 0.090–0.910 mg/l, hematological effect; Salmo gairdneri, 2 d, 9.1 mg/l, lethal effect (Heming & Blumhagen 1988). Salvelinus fontinalis, 45–60 d, 0.283 mg/l, growth effect; mortality (Hunn et al. 1987b).	

78 • Amberlite LA1 * 12642-13-6

Chemicals in the product	Aliphatic amines	
EC50 values to algae, mg/l	0.021 0.057	5d, rpd, Asterionella formosa 5d, rpd, Selenastrum capricornutum (Blanck 1984)
LC50 values to fishes, mg/l	1.2–6.4	120 hr, Salmo gairdneri (Dave et al. 1979)

79 • Ambush * 52645-53-1

Active ingredients	Permethrin * 250 g/l	
LC50 values to crustaceans, mg/l	0.0006	96 hr, 21 °C, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	0.004–0.008	96 hr, 10 °C, Alburnus alburnus (Linden et al. 1979)

80 • Ametryn 834-12-8

Synonyms	2-Ethylamino-4-isopropylamino-6-methylthio-1,3,5-triazine 2-Ethylamino-4-isopropylamino-6-methylmercapto-s-triazine 2-Ethylamino-4-isopropylamino-6-methylthio-s-triazine 6-Ethylamino-4-isopropylamino-2-methylthio-1,3,5-triazine	
Use	Herbicide.	
State and appearance	Colourless crystals.	
Vapour pressure, mmHg	0.00000084 mmHg, 20 °C	
Melting point, °C	84–85	
Log soil sorption coefficient, log Kom	2.59	(Sabljic 1987)
LD50 values to mammals in oral exposure, mg/kg	1110	technical, orl-rat (Anon. 1976)
LD50 values to mammals in non-oral exposure, mg/kg	> 8160	skn-rbt (Martin 1968)
Other information about mammals	In diet: rats fed ninety days at 100 mg/kg/day were comparable to controls except for slight histological changes in the liver (Martin 1968).	
Effects on plants	Soil was amended to give 2.0 ppm by weight of soil of ametryn —atrazine-susceptible lamb's-quarters (Chenopodium album L.) were killed soon after germination and emergence (Jensen et al. 1977).	
EC50 values to algae, mg/l	0.01 0.01	rpd, schr, Chlorococcum sp. pht, schr, Isochyris galbana Phaeodactylum tricornutum (Walsh 1972)
EC50 values to crustaceans, mg/l	40	2d (Marchini et al. 1988)

Other information about water organisms	Algae: Chlorococcum sp. (technical acid): 20 ppb: 50% decrease in 02 evolution Chlorococcum sp.: 10 ppb: 50% decrease in growth; measured as ABS (525 mu) after 10 days Dunaliella tertiolecta: 40 ppb: 50% decrease in 02 evolution 50% decrease in growth; measured as ABS (525 mu) after 10 days Isochrysis galbana: 10 ppb: 50% decrease in 02 evolution 50% decrease in growth; measured as ABS (525 mu) after 10 days Phaeodactylum tricornutum: 10 ppb: 50% decrease in 02 evolution Phaeodactylum tricornutum: 20 ppb: 50% decrease in growth; measured as ABS (525 mu) after 10 days (Walsh 1972).

81 • 3-Amino-2,5-dichlorobenzoic acid 133-90-4

Use	Selective preemergence herbicide.	
State and appearance	White odourless chrystalline solid.	
Odour	Odourless.	
Vapour pressure, mmHg	0.007	at 100 °C
Melting point, °C	200–201	
LD50 values to mammals in oral exposure, mg/kg	5620	as free acid, orl-male albino rats (Verschueren 1983)
LD50 values to mammals in non-oral exposure, mg/kg	3160	skn-albino rats (Verschueren 1983)
EC50 values to algae, mg/l	50 50 15 25	rpd, schr, 10 d, Chlorococcum sp. rpd, schr, 10 d, Dunaliella terticulata rpd, schr, 10 d, Isochrysis galbana rpd, schr, 10 d, Phaeodactylum tricornutum (Walsh 1972)
Other information about water organisms	Technical acid: 115000 ppb: 50000 ppb: Technical acid: 115000 ppb: 50000 ppb: Technical acid: 100000 ppb: 15000 ppb: Technical acid: 100000 ppb: 25000 ppb:	Chlorococcum sp.: 50% decrease in 02 evolution 50% decrease in growth (measured as ABS (525 mu) after 10 days) Dunaliella tertiolecta: 50% decrease in 02 evolution 50% decrease in growth (measured as ABS (525 mu) after 10 days) Isochrysis galbana: 50% decrease in 02 evolution 50% decrease in growth (measured as ABS (525 mu) after 10 days) Phaeodactylum tricornutum: 50% decrease in 02 evolution 50% decrease in growth (measured as ABS (525 mu) after 10 days)

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	Ammonium salt: 2225000 ppb: 4000000 ppb:	Chlorococcum sp.: 50% decrease in 02 evolution 50% decrease in growth (measured as ABS (525 mu) after 10 days)
	Ammonium salt: 2750000 ppb: 4000000 ppb:	Dunaliella tertiolecta: 50% decrease in 02 evolution 50% decrease in growth (measured as ABS (525 mu) after 10 days)
	Ammonium salt: 1500000 ppb: 3500000 ppb:	Isochrysis galbana: 50% decrease in 02 evolution 50% decrease in growth (measured as ABS (525 mu) after 10 days) (Walsh 1972).
Other information	Ammoniumsalts approximately 100 X less toxic (Walsh 1972).	

82 • 3-Amino-2,4-dinitrotoluene 70343-06-5

EC50 values to crustaceans, mg/l	8.1	mbt, 48 hr, Daphnia magna (Pearson et al. 1979)
LC50 values to fishes, mg/l	12.2	96 hr, Pimephales promelas (Pearson et al. 1979)

83 • 5-Amino-2,4-dinitrotoluene 5267-27-6

EC50 values to crustaceans, mg/l	3.1	mbt, 48 hr, Daphnia magna (Pearson et al. 1979)
LC50 values to fishes, mg/l	2.4	96 hr, Pimephales promelas (Pearson et al. 1979)

84 • 3-Amino-2,6-dinitrotoluene 10202-92-3

Synonyms	5-Methyl-4,6-dinitrobenzenamine	
EC50 values to crustaceans, mg/l	4.7	mbt, 48 hr, Daphnia magna (Pearson et al. 1979)
LC50 values to fishes, mg/l	11.3	96 hr, Pimephales promelas (Pearson et al. 1979)

85 • 4-Amino-2,6-dinitrotoluene 19406-51-0

EC50 values to crustaceans, mg/l	5.2	mbt, 48 hr, Daphnia magna (Pearson et al. 1979)
LC50 values to fishes, mg/l	6.9	96 hr, Pimephales promelas (Pearson et al. 1979)

86 • 1-Amino-2-methoxy-5-methylbenzene 120-71-8

Melting point, °C	93–94	(MITI 1992)
Boiling point, °C	235	(MITI 1992)

Total degradation in water	Biodegradation: 0.7% by BOD period:14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).	
Bioconcentration factor, fishes	< 4.6 < 25	6w, Cyprinus carpio, conc 2 mg/l 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	170	48 hr, Oryzias latipes (MITI 1992)

87 • 4-Amino-2-nitrophenol 119-34-6

LC50 values to fishes, mg/l	34.3	96 hr, Pimephales promelas (Holcombe et al. 1984)

88 • 4-Amino-2-nitrotoluene 89-62-3

EC50 values to crustaceans, mg/l	14.2	48 hr, mbt, Daphnia magna (Pearson et al. 1979)
LC50 values to fishes, mg/l	26.1	96 hr, Pimephales promelas (Pearson et al. 1979)

89 • 1-Amino-2-propanole 78-96-6

Synonyms	Monoisopropanolamine	
LC50 values to fishes, mg/l	> 5000	Carassius auratus (Bridie et al. 1979)

90 • 2-Amino-3,5-diiodobenzoic acid 609-86-9

Other information about degradation	Impact on biodegradation processes: at 100 mg/l no inhibition of NH3 oxidation bu Nitrosomonas sp. (Hockenbury & Grady 1977).

91 • 4-Amino-3,5-dinitrotoluene 6393-42-6

EC50 values to crustaceans, mg/l	> 13.1	mbt, 48 hr, Daphnia magna (Pearson et al. 1979)
LC50 values to fishes, mg/l	> 13.1	96 hr, Pimephales promelas (Pearson et al. 1979)

92 • 4-Amino-3,5-xylenol 3096-70-6

LC50 values to fishes, mg/l	0.32	96 hr, Lepomis macrochirus (Mauck et al. 1977)

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93 • 2-Amino-3,6-dinitrotoluene 56207-39-7

EC50 values to crustaceans, mg/l	2.2	mbt, 48 hr, Daphnia magna (Pearson et al. 1979)
LC50 values to fishes, mg/l	0.78	96 hr, Pimephales promelas (Pearson et al. 1979)

94 • 2-Amino-4,6-dinitrotoluene 35572-78-2

EC50 values to crustaceans, mg/l	4.5	mbt, 48 hr, Daphnia magna (Pearson et al. 1979)
LC50 values to fishes, mg/l	14.8	96 hr, Pimephales promelas (Pearson et al. 1979)

95 • 7-Amino-4-hydroxy-2-naphthalene sulfonic acid 87-02-5

Total degradation in water	Biodegradation: 6.3% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.2 < 2.4	6w, Cyprinus carpio, conc 2 mg/l 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	480	48 hr, Oryzias latipes (MITI 1992)

96 • 1-Amino-4-nitronaphthalene 776-34-1

Other information about water organisms	EC50, 60 hr, 15 mg/l, rpd, Tetrahymena pyriformis (Schultz & Applehans 1985).

97 • 2-Amino-4-nitrotoluene 119-32-4

EC50 values to crustaceans, mg/l	22.5	mbt, 48 hr, Daphnia magna (Pearson et al. 1979)
LC50 values to fishes, mg/l	34 71.3	96 hr, Pimephales promelas (Holcombe et al. 1984) 96 hr, Pimephales promelas (Pearson et al. 1979)

98 • 3-Amino-4-nitrotoluene 578-46-1

EC50 values to crustaceans, mg/l	5.8	mbt, 48 hr, Daphnia magna (Pearson et al. 1979)
LC50 values to fishes, mg/l	25.5	96 hr, Pimephales promelas (Pearson et al. 1979)

99 • 4-Amino-5-carbamoylimidazole salt of hydrochloric acid 72-40-2

Sumformula of the chemical	C4H6N4O.ClH	
EINECS-number	2007783	
Water solubility, mg/l	> 10000 (MITI 1992)	
Total degradation in water	Biodegradation: 0–12% by BOD period: 28d substance: 100 mg/l sludge: 100 mg/l (MITI 1992).	
Bioconcentration factor, fishes	0.7–1.6 7.9–17	6w, Cyprinus carpio, conc 2 mg/l 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 500	48 hr, Oryzias latipes (MITI 1992)

100 • 2-Amino-5-chloro-4-methylbenzene sulfonic acid 88-53-9

Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).	
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	> 1000	48 hr, Oryzias latipes (MITI 1992)

101 • 2-Amino-5-guanidopentanoic acid 74–79–3

Synonyms	dl-Arginine	
Sumformula of the chemical	NH2C(NH)NH(CH2)3CH(NH2)COOH	
Use	Biochemical research; medicine; pharmaceuticals; natural sources; widely found in animal and plant proteins.	
Molecular weight	174.21	
Water solubility, mg/l	150000	l-arginine
Boiling point, °C	238	l-arginine
Degradation point, °C	217–218	
Log octanol/water coefficient, log Pow	-2.59	calculated
Other information about degradation	Impact on biodegradation processes: approximately 50% inhibition of NH3 oxidation in Nitrosomonas at 1.7 mg/l (l-isomer) (Verschueren 1983).	

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102 • 2-Amino-5-methylbenzenesulfonic acid 88-44-8

Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.4 < 4.0	6w, Cyprinus carpio, conc 2 mg/l 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	480	48 hr, Oryzias latipes (MITI 1992)

103 • 2-Amino-5-nitropyridine 4214-76-0

Other information about water organisms	EC50, 60 hr, 83 mg/l, rpd, Tetrahymena pyriformis (Schultz & Applehans 1985).

104 • 5-Amino-6-nitroquinoline 35975-00-9

Other information about water organisms	EC50, 60 hr, 23 mg/l, rpd, Tetrahymena pyriformis (Schultz & Applehans 1985).

105 • 2-Amino-6-nitrotoluene 570-24-1

EC50 values to crustaceans, mg/l	13.2	mbt, 48 hr, Daphnia magna (Pearson et al. 1979)
LC50 values to fishes, mg/l	49.9	96 hr, Pimephales promelas (Pearson et al. 1979)

106 • 1-Amino-8-naphthol-3,6-disulfonic acid monosodium salt 5460-09-3

Sumformula of the chemical	C10H7O7NSNa	
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.3 < 2.9	6w, Cyprinus carpio, conc 2 mg/l 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
LC50 values to fishes, mg/l	880	48 hr, Oryzias latipes (MITI 1992)

107 • 2-Amino-8-naphthol-6-sulfonic acid 90-51-7

Sumformula of the chemical	C10H9NO4S
EINECS-number	2020008
Total degradation in water	Biodegradation: 5.3% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.1–0.5 6w, Cyprinus carpio, conc 1 mg/l < 1.0–7.1 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
LC50 values to fishes, mg/l	335 48 hr (MITI 1992)

108 • 4-Amino-m-toluenesulfone acid 98-33-9

LC50 values to fishes, mg/l	375 96 hr, Gambusia affinis (Jones 1971)

109 • Aminoacetic acid 56-40-6

Synonyms	Aminoethanoic acid Glycine Glycocoll
Sumformula of the chemical	H2NCH2COOH
Use	Stabilizing agent in photo processing. Organic synthesis, nutrient, buffering agent.
State and appearance	Crystalline.
Molecular weight	75.07
Specific gravity (water=1)	1.601
Water solubility, mg/l	253000 at 25 °C 575000 at 75 °C
Degradation point, °C	233 melting point 289 boiling point
Effects on wastewater treatment	Impact on conventional biological treatment systems: unacclimated system at 500 mg/l: biodegradable (Verschueren 1983).
Other information	Natural sources: normal constituent of proteins Manmade sources; excreted by man in urine: 2.3 to 18 mg/kg body weight/day (Verschueren 1983).

110 • 2-Aminoanthracene 613-13-8

Sumformula of the chemical	C14H11N
pKa	4.1 (Sangster 1989)
Log octanol/water coefficient, log Pow	3.4 (Sangster 1989)
Log soil sorption coefficient, log Kom	4.45 observed (Sabljic 1987) 4.48 calculated (Sabljic 1987)

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Effects on the physiology of water organisms	Salmo gairdneri: 0.63 mmol, 6 days –biochemical e ffect (change in physio-chemical process including glycogen uptake, cholesterol levels and lipid analysis) (Miyauchi & Uematsu 1987).

111 • 1-Aminoanthraquinone

82-45-1

Sumformula of the chemical	C14H9NO2
EINECS-number	2014235
Water solubility, mg/l	0.32 (MITI 1992)
Melting point, °C	256–258 (MITI 1992)
Log octanol/water coefficient, log Pow	3.74 (MITI 1992)
Total degradation in water	Biodegradation: 0–1% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	50–150 8w, Cyprinus carpio, conc 0.03 mg/l 55–137 8w, Cyprinus carpio, conc 0.003 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 30.0 Oryzias latipes (MITI 1992)

112 • 2-Aminoanthraquinone

117-79-3

Synonyms	9,10-Anthracenedione, 2-amino-
Sumformula of the chemical	C14H9NO2
EINECS-number	2042084
Water solubility, mg/l	0.15 (MITI 1992)
Melting point, °C	299 (MITI 1992)
Log octanol/water coefficient, log Pow	3.31 (MITI 1992)
Total degradation in water	Biodegradation: 0–2% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	27–43 6w, Cyprinus carpio, conc 0.05 mg/l 18–46 6w, Cyprinus carpio, conc 0.005 mg/l (MITI 1992)
LC50 values to fishes, mg/l	30 48 hr, Oryzias latipes (MITI 1992)

113 • 2-Aminobenzimidazole

934-32-7

Sumformula of the chemical	C7H7N3
Use	In photographic industry as an antifoggant.

Molecular weight	133.15
Melting point, °C	229–231
Aerobic degradation in soil	Biodegradation: total evolution of 14C in CO2 and remaining radio-activity in soil after 218 days of incubation at 25 °C with 4 ppm 14C-2 amino-benzimidazole *not inoculated* / *inoculated with adapted soil* 14C-evolution 48.2% 84.2–84.3% 14C-soil residues 40.6% 10.7–18.0% % recovery 88.8% 94.9–102.3% (Verschueren 1983).
LD50 values to mammals in oral exposure, mg/kg	600 orl-mus (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	100 ipr-mus 126 ivn-mus (Sweet 1987)
LDLo values to mammals in oral exposure, mg/kg	500 orl-rat (Sweet 1987)
TDLo values to mammals in oral exposure, mg/kg	426 orl-rat, 8-15d preg. effects on embryo of fetus (Sweet 1987)
Mutagenicity	Mutation data: microbial muation withour S9: S. typhimurium; 0.1 mg/plate; microsomal assay: S. typhimurium; 0.710 mg/l (Sweet 1987).
Other information about water organisms	EC50, 60 hr, 120 mg/l, rpd, Tetrahymena pyriformis (Schultz & Applehans 1985).
Other information	Manmade source; degradation product (hydrolysis) of the fungicides benomyl, carbendazim, and thiophanate methyl (Verschueren 1983).

114 • m-Aminobenzoic acid

99-05-8

Synonyms	3-Carboxyaniline
Molecular weight	137.13
Specific gravity (water=1)	1.511 at 20/4 °C
Water solubility, mg/l	5900 at 15 °C
Melting point, °C	174
Total degradation in soil	Biodegradation: decomposition by a soil microflora: > 64 days (Verschueren 1983).
LD50 values to birds in oral exposure, mg/kg	750 orl-Agelaius phoeniceus > 1000 orl-Sturnus vulgaris > 1000 orl-Coturnix coturnix > 1000 orl-Passer domesticus (Schafer et al. 1983)

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115 • o-Aminobenzoic acid 118-92-3

Synonyms	Anthranilic acid
Use	Dyes; drugs; perfumes; pharmaceuticals.
Molecular weight	137.13
Water solubility, mg/l	3500 at 14 °C
Melting point, °C	145–147
Log octanol/water coefficient, log Pow	1.21
Total degradation in soil	Decomposition period by a soil micro flora: 2 days (Verschueren 1983).
Other information about degradation	Lag period for degradation of 16 mg/l by waste water or by soil at pH 7.3 and 30 °C: less than 1 day (Haller 1978). Impact on biodegradation processes: at 100 mg/l no inhibition of NH3 oxidation by Nitrosomonas sp. (Hockenbury & Grady 1977).
LD50 values to birds in oral exposure, mg/kg	750 orl-Agelaius phoeniceus > 1000 orl-Sturnus vulgaris > 1000 orl-Coturnix coturnix > 1000 orl-Passer domesticus (Schafer et al. 1983)

116 • p-Aminobenzoic acid 150-13-0

Synonyms	4-Carboxyaniline
Molecular weight	137.13
Water solubility, mg/l	3400 at 9.6 °C
Melting point, °C	187
Log octanol/water coefficient, log Pow	0.68
Total degradation in soil	Biodegradation: decomposition by a soil microflora: > 8 days (Verschueren 1983). Lag period fo degradation of 16 mg/l by wastewater or by soil at pH 7.3 and 30 °C: less than 1 day (Verschueren 1983).
Other information about degradation	Impact on biodegradation processes: at 100 mg/l no inhibition of NH3 oxidation by Nitrosomonas sp. (Verschueren 1983).
LD50 values to birds in oral exposure, mg/kg	> 1000 orl-Agelaius phoeniceus > 1000 orl-Sturnus vulgaris > 1000 orl-Coturnix coturnix > 1000 orl-Passer domesticus (Schafer et al. 1983)

117 • 3-Aminobenzoic acid ethyl ester methanesulfonate 886-86-2

Synonyms	MS-222 Tricainemethanesulfonate Ethyl m-aminobenzoate, methanesulfonic acid salt Ethyl m-aminobenzoate methane sulfonate Tricaine Tricaine methane sulfonate

Sumformula of the chemical	C10H15N05S	
Molecular weight	261.32	
LD50 values to mammals in non-oral exposure, mg/kg	180	ivn-mus (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	> 100 > 100	orl-Agelaius phoeniceus orl-Sturnus vulgaris (Schafer et al. 1983)
LC50 values to fishes, mg/l	50.5	4d, Salmo gairdneri (McKim et al. 1987)
LOEC values to fishes, mg/l	25	3 hr, phy, Oncorhynchus kisutch (Strange & Schreck 1978)
Other information about water organisms	Lethal threshold concentration (LT50): 50.2 mg/l, 0.2 d, Salmo gairdneri (McKim et al. 1987).	

118 • Aminocarb 2032-59-9

Synonyms	4-(Dimethylamino)-3-methylphenyl-N-methylcarbamate(ester) 4-Dimethylamino-m-tolylmethylcarbamate	
Use	Nonsystemic insecticide, molluscicide.	
State and appearance	White crystalline solid.	
Molecular weight	208.29	
Melting point, °C	93–94	
Total degradation in water	Persistence in river water in a sealed glass jar under sunlight and artificial fluorescent light - initial concentration 0.010 mg/l: *% of original compound found* after: 1 hr — 100; 1 wk — 60; 2 wks — 10; 4 wks — 0; 8 wks — 0 (Eichelberger & Lichtenberg 1971).	
Bioconcentration factor, mollusca	3.8–4.9	Mytilus edulis, on wet weight (McLeese et al. 1980)
LD50 values to mammals in oral exposure, mg/kg	30 50	orl-rat (Lewis & Sweet 1984) orl-rat (Ames et al. 1973)
LD50 values to mammals in non-oral exposure, mg/kg	275 21 275	skn-rat (Lewis & Sweet 1984) ipr-rat (Ames et al. 1973) skn-rat (Ames et al. 1973)
Other information about mammals	ALD = 94.0 mg/kg, act, orl, deer mouse; LDfr = 100 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987). In diet: rats fed 5 mg/kg/day for twenty-eight days showed no symptoms of poisoning (Ames et al. 1973).	
LD50 values to birds in oral exposure, mg/kg	23 50 50 100–212	orl-dck orl-bwd (Lewis & Sweet 1984) orl-Agelaius phoeniceus orl-Sturnus vulgaris (Schafer et al. 1983)
Effects on invertebrates	LC50, 2 days: 0.478 mg/l, Ophiogomphus sp. 0.590 mg/l, Pycnopsyche sp. 2.863 mg/l, Simulium venustum (Poirier & Surgeoner 1987).	

Effects on arthropods	Fourth instar larval Chironomus riparius: LC50 24 hr: 376.6 ppb (Estenik & Collins 1979).	
EC50 values to algae, mg/l	0.1	24hr, rpd, Selenastrum capricornutum (Corture et al. 1982)
LOEC values to algae, mg/l	0.1	24 hr, Selenastrum capricornutum (Corture et al. 1982)
LC50 values to crustaceans, mg/l	0.012 1.184	96 hr, Gammarus lacustris (Sanders 1969) 6 hr, Orconectes sp. delayed effect in recovery water (Poirier & Surgeoner 1988)
LC50 values to fishes, mg/l	0.09 8.7 3.5 26 49–60	96 hr, Salmo clarki (Woodward & Mauck 1980) 96hr, Salmo salar 96hr, Salmo salar (McLeese et al. 1980) 96hr, Salmo clarci (Woodward & Mauck 1980) 0.13d, Salmo gairdneri (Doe et al. 1988)
Effects on the physiology of water organisms	Salmo gairdneri; 0.13 d, 10 mg/l, enzyme effect (Doe et al. 1988). Simulium sp., delayed effect in recovery water, LC50, 6 hr, 0.344 mg/l (Poirier & Surgeoner 1988).	
Other information about water organisms	LC50, 6 hr, delayed effect in recovery water: Isonychia sp., 0.478 mg/l; Acroneuria sp., 1.062 mg/l; Ophiogomphus sp., 1.017 mg/l; Pycnopsyche sp., 1.276 mg/l (Poirier & Surgeoner 1988).	

119 • p-Aminodimethylaniline 99-98-9

Synonyms	Dimethylaminoaniline Dimethyl-p-phenylenediamine
Use	Base for production of methyleneblue; photodeveloper; reagent for cellulose.
State and appearance	Colourless, asbestos-like needles.
Melting point, °C	41
Boiling point, °C	257
Other information about water organisms	Green algae: Microcystis aeruginosa: LD100: 2 ppm (Verschueren 1983).

120 • 2-Aminoethanol 141-43-5

Synonyms	Monoethanol amine β -Aminoethyl alcohol Ethanol amine β -Ethanolamine Glycinol 2-Hydroxyethylamine β -Hydroxyethylamine Colamine
Sumformula of the chemical	C2H7NO
Use	Solvent. Mordant manufacture; manufacture pharmaceuticals; chemicals production; fertilizers.
State and appearance	Colourless.

Melting point, °C	10.5 (MITI 1992)
Boiling point, °C	170.95 (MITI 1992)
Volatilization	Relative volatility (nBuAc=1) = 0.05
Chemical oxygen demand, g 02/g	1.28 5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.93 5 days (Bridie et al. 1979)
Total degradation in water	Biodegradation: 49% by BOD (on the upward trend) period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	2100 orl-rat (Lewis & Sweet 1984) 3320 orl-rat 2149 orl-rat 10200 14d, orl-rat 2050 orl-rat 1475 orl-mus 1000 orl-rbt 620 orl-gpg (Sax 1986)
LD50 values to mammals in non-oral exposure, mg/kg	981 ipr-rat 800 ivn-rat 2537 scu-mus 1000 skn-rbt (Lewis & Sweet 1984)
Health effects	Irritant. Moderately toxic with ingestion or inhalation. Emits toxic vapours when heated to decomposition (Sax 1986).
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 6300 mg/l (Bringmann & Kühn 1980a)
LOEC values to algae, mg/l	1.6 rpd, schr, Microcystis aeruginosa 0.75 rpd, schr, Scenedesmus quadricauda Bringmann & Kühn 1980a
LC50 values to crustaceans, mg/l	> 100 48 hr, brine shrimp (Sax 1986)
LC50 values to fishes, mg/l	> 5000 24 hr, Carassius auratus (Bridie et al. 1979)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 0.75 mg/l protozoa (Entosiphon sulcatum): 300 mg/l (Bringmann & Kühn 1980a)
Other information	Air pollution: high (Sax 1986).

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121 • 2-(2-Aminoethylamino)ethanol 111-41-1

Boiling point, °C	242.0–246.0 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.2 6w, Cyprinus carpio, conc 1 mg/l < 2.1–3.7 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	> 1000 mg/l, 48 hr, Oryzias latipes (MITI 1992)

122 • Aminoglycol 115-69-5

Other information about mammals	LDfr = 100 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

123 • 5-Aminoindazole 5401-94-5

Other information about water organisms	EC50, 60 hr, 46 mg/l, rpd, Tetrahymena pyriformis (Schultz & Applehans 1985).

124 • 5-Aminoindole 5192-03-0

Other information about water organisms	EC50, 60 hr, 150 mg/l, rpd, Tetrahymena pyriformis (Schultz & Applehans 1985).

125 • 6-Aminonicotinamide 329-89-5

Other information about mammals	ALD = 94.0–320.0 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987).

126 • 3-Aminoquinoline 580-17-6

Other information about water organisms	EC50, 60 hr, 170 mg/l, rpd, Tetrahymena pyriformis (Schultz & Applehans 1985).

127 • 5-Aminoquinoline 611-34-7

Other information about water organisms	EC50, 60 hr, 240 mg/l, rpd, Tetrahymena pyriformis (Schultz & Applehans 1985).

128 • m-Aminophenol 591-27-5

Synonyms	3-Aminophenol m-Hydroxyaniline
Use	Dye intermediate.
Molecular weight	109.12
Water solubility, mg/l	26000
Melting point, °C	120–122 (MITI 1992)
Log octanol/water coefficient, log Pow	0.16
Total degradation in soil	Biodegradation: decomposition by a soil microflora: > 64 days (Verschueren 1983).
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 30mg/l sludge: 100 mg/l (MITI 1992).
Other information about degradation	Lag period for degradation of 16 mg/l by waste water and soil suspension at pH 7.3 and 30 °C: > 25 days (Haller 1978). Impact on biodegradation processes: at 0.6 mg/l, inhibition of degradation of glucose by Pseudomonas fluorescens; at 9 mg/l, inhibion of degradation of glucose by E. coli (Bringmann & Kühn 1960).
Bioconcentration factor, fishes	< 4 6w, Cyprinus carpio, conc 1 mg/l < 40 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to birds in oral exposure, mg/kg	237 orl-Agelaius phoeniceus > 1000 orl-Sturnus vulgaris 750 orl-Coturnix coturnix > 1000 orl-Passer domesticus (Schafer et al. 1983)
LC50 values to fishes, mg/l	100 48hr, Oryzias latipes (MITI 1992)
Other information about water organisms	Algae: Chlorella pyrenoidosa: toxic at 140 mg/l (Jones 1971).

129 • o-Aminophenol 95-55-6

Synonyms	o-Hydroxyaniline
Molecular weight	109.12
Water solubility, mg/l	17000 at 0 °C
Melting point, °C	172
Log octanol/water coefficient, log Pow	0.52–0.62
Total degradation in soil	Decomposition period by a soil microflora: 4 days (Verschueren 1983).

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LD50 values to birds in oral exposure, mg/kg	> 1000 orl-Agelaius phoeniceus > 1000 orl-Sturnus vulgaris 316 orl-Coturnix coturnix 316 orl-Passer domesticus (Schafer et al. 1983)
Other information about water organisms	Algae: Chlorella pyrenoidosa: 47 mg/l: toxic (Jones 1971).

130 • p-Aminophenol 123-30-8

Synonyms	p-Hydroxyaniline 4-Aminophenol 4-Amino-1-hydroxybenzene
Use	Photograph developing.
Molecular weight	109.12
Water solubility, mg/l	11000 at 0 °C
Degradation point, °C	184
Log octanol/water coefficient, log Pow	0.04
Carcinogenicity	Carcinogenicity: negative (McCann et al. 1975).
Mutagenicity	Mutagenicity in the Salmonella test: neg; < 0.01 revertant colonies/nmol; < 70 revertant colonies at 0.5 mg/plate (McCann et al. 1975).
LD50 values to birds in oral exposure, mg/kg	56.2 orl-Agelaius phoeniceus > 1000 orl-Sturnus vulgaris > 1000 orl-Coturnix coturnix 178 orl-Passer domesticus (Schafer et al. 1983)
Effects on microorganisms	Bacteria: Escherichia coli: toxic: 8–10 mg/l (Jones 1971).
LC50 values to fishes, mg/l	24 96hr, Pimephales promelas (Vincent et al. 1976)
Other information about water organisms	Algae: Chlorella pyrenoidosa; toxic at 140 mg/l (Jones 1971) Scenedesmus: toxic at 6 mg/l (Meinck et al. 1970). Arthropoda: Daphnia: toxic: 0.6 mg/l (Meinck et al. 1970). Fish: goldfish: approx. fatal conc.: 2.0 mg/l; 48hr (McKee & Wolf 1963).

131 • (4-Aminophenyl)arsonic acid 98-50-0

Effects on the physiology of water organisms	Salmo gairdneri, 56 d, 1.6 mg/l, growth effect (Cockell & Hilton 1988).

132 • 2-Aminopyridine 504-29-0

Synonyms	α-Pyridylamine
Molecular weight	94.11
Vapour density (air=1)	3.25
Conversion factor, 1 ppm in air=	3.91 mg/m^3

Conversion factor, 1 mg/m³ in air=	0.26 ppm
Water solubility, mg/l	> 4000 (MITI 1992)
Melting point, °C	56–61 (MITI 1992)
Boiling point, °C	204 (MITI 1992)
Log octanol/water coefficient, log Pow	-0.22 0.6 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	3.0–7.7 6w, Cyprinus carpio, conc 0.1 mg/l < 5.1–25 6w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	200 orl-rat 50 orl-mus (Patty 1967)
Health effects	Man: readily absorbed through the skin transient symptoms: 5.2 ppm, 8 hours (Patty 1967).
LD50 values to birds in oral exposure, mg/kg	31.6 orl-Agelaius phoeniceus 75.0–100 orl-Sturnus vulgaris 133 orl-Coturnix coturnix 75 orl-Passer domesticus (Schafer et al. 1983)
LC50 values to fishes, mg/l	10 48 hr, Oryzias latipes (MITI 1992)
Other information about water organisms	EC50, 60 hr, 390 mg/l, rpd, Tetrahymena pyriformis (Schultz & Applehans 1985). EC50, 2.5 days, 393 mg/l, grw, Tetrahymena pyriformis (Schultz et al. 1987).

133 • 3-Aminopyridine 462-08-8

Synonyms	3-Pyridinamine β-Aminopyridine Amino-3 pyridine m-Aminopyridine 3-Pyridylamine
Sumformula of the chemical	C5H6N2
Molecular weight	94.13
Water solubility, mg/l	> 5000 (MITI 1992)
Melting point, °C	64 (MITI 1992)
Boiling point, °C	250–252 (MITI 1992)

Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.2 6w, Cyprinus carpio, conc 0.2 mg/l < 2.1 6w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in non-oral exposure, mg/kg	4 intracerebral-mus 28 ipr-mus 24 ivn-mus 30 scu-mus (Sweet 1987)
LD50 values to birds in oral exposure, mg/kg	13.3 orl-bdw 178 orl-qal (Sweet 1987) 13.3 orl-Agelaius phoeniceus 133 orl-Sturnus vulgaris 178 orl-Coturnix coturnix 133 orl-Passer domesticus (Schafer et al. 1983)
LC50 values to fishes, mg/l	8.1 48 hr, Oryzias latipes (MITI 1992)
Other information about water organisms	Tetrahymena pyriformis, EC50, grw, 2,5 d, 283.0 mg/l (Schultz et al. 1987).

134 • 4-Aminopyridine 504-24-5

Synonyms	4-Pyridinamine gamma-Aminopyridine p-Aminopyridine 4-Pyridylamine
Sumformula of the chemical	C5H6N2
Purity, %	97, 98, 95
Use	Intermediate. Used as a bird repellent and poison. The distress calls of poisoned individuals warn other members of the flock to leave the place. It is used in agriculture, in urban areas to control pigeons and sparrows, and in airports to keep out seagulls.
State and appearance	A solid with a tan to brown colour.
Molecular weight	94.12
Water solubility, mg/l	83000 25 °C 76600 25 °C > 10000 (MITI 1992)
Melting point, °C	155–158 (MITI 1992)
Boiling point, °C	273.5
Flashing point, °C	164
Log octanol/water coefficient, log Pow	0.28

Adsorption/desorption	Readily adsorbed by soil colloids (Sax 1986).
Other physico–chemical properties	Flammability: Some of these materials may burn but do not ignite readily. 4-aminopyridine is a strong base.
Aerobic degradation in soil	Degradation of 4-aminonopyridine-14C to 14C02: under aerobic incubation, after 3 months at 30 °C and 50% moisture, evolution of 14C02 ranged from 0.4% for a highly acidic loam (pH 4.1) to more than 50% for a lighter-textured, alkaline, loamy sand (pH 7.8) (Starr & Cunningham 1975).
Anaerobic degradation in soil	Degradation of 4-aminonopyridine-14C to 14C02: was neglible in soils incubated up to 2 months under anaerobic conditions (Starr & Cunningham 1975).
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.2–0.6 6w, Cyprinus carpio, conc 0.05 mg/l < 1.8–7.2 6w, Cyprinus carpio, conc 0.005 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	20 orl-rat (Sax 1986)
LD50 values to mammals in non-oral exposure, mg/kg	6.5 ipr-rat 19 scu-rat 10 ipr-mus 7 ivn-mus 5.5 ivn-rbt 10.13 scu-rat 11.9 scu-mus (Sax 1986)
LDLo values to mammals in oral exposure, mg/kg	0.59 orl-man 28 orl-rat 4 orl-dog 18 orl-pig (Sax 1986)
LDLo values to mammals in non-oral exposure, mg/kg	5 scu-mus 327 skn-rbt (Sax 1986)
Other information about mammals	ALD = 42.0 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987).
Health effects	Direct contact: Irritates eyes, skin, and mumem. Aminopyridines penetrate guinea pig skin readily. One employee died after spilling an analog of 4-aminopyridine on his clothes during its distillation and continuing to work in them for 1.5 hr. General sensation: Symptoms for aminopyridines; convulsions, dizziness, dyspnea, headache, hypertension, nausea and vomiting, weakness. Pyridine compounds as a class cause anorexia, nausea, weakness, dizziness, and headache. Acute hazard level: Highly oral toxicity. Causes noticeable central nervous system depression (Sax 1986).

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LD50 values to birds in oral exposure, mg/kg	7.65	orl- Coturnix quail
	7.5	orl- Common pigeon
	7.5	orl- House sparrow
	4.9	orl- Starling
	2.37	orl- Common grackle
	2.37	orl- Redwinged blackbird (Sax 1986)
	1.78–8.50	orl-Agelaius phoeniceus
	4.9	orl-Sturnus vulgaris
	7.65–8.05	Coturnix coturnix
	3.80–7.50	orl-Passer domesticus
	2.37	orl-Quiscalus quiscula
	7.5	orl-Columba livia
	5.62	orl-Carpodacus mexicanus
	4.22	orl-Anas platyrhynchos
	5.62–7.50	orl-Phasianus colchicus
	5.62	orl-Falco sparverius
	10	orl-Volatia jacarina
	2.37	orl-Pica pica
	4.22	orl-Molothrus ater
	3.16	orl-Tangavius aeneus
	2.37–3.16	orl-Cassidix major
	10	orl-Aratinga pertinax
	5.62	orl-Melopsittacus undulatus
	2.37	orl-Corvus brachyrhynchos
	10	orl-Spiza americana
	5.62	orl-Zonotrichia atricapilla
	2.37–2.74	orl-Passer luteus
	8.10–8.50	orl-Zenaida macroura
	12	orl-Myiopsitta monachus
	4.22–4.87	orl-Ploceus taeniopterus
	12	orl-Aratinga canicularis
	1.78–2.37	orl-Euplectes orix
	5.62	orl-Quelea quelea
	< 7.2	orl-Sporophila minuta
	< 1.00	orl-Molothrus bonariensis
	4.22	orl-Agelaius tricolor
	2.37	orl-Pica nuttalli (Schafer et al. 1983)
LC50 values to fishes, mg/l	2.82–7.56	srv, act, 96 hr, Lepomis macrochirus (Schafer & Marking 1975)
	2.43–5.80	srv, act, 96 hr, Ictalurus punctatus (Schafer & Marking 1975)
	2.65	48 hr, Oryzias latipes (MITI 1992)
Other information about water organisms	EC50, 60 hr, 260 mg/l, rpd, Tetrahymena pyriformis (Schultz & Moulton 1985).	

135 • Amitrole

61-82-5

Synonyms	3-Amino-1,2,4-triazole Aminotriazole ATA Amerol 2-Aminotriazole 3-Aminotriazole 3-Amino-s-triazole 2-Amino-1,3,4-triazole Amitol Amitril Amitrol Amitrole Fenamine Simazol Triazolamine Weedazin Weedazol
Sumformula of the chemical	C2H4N4
Purity, %	90
Known impurities	Ammonium thiocyanateatrazinebromacillinuronsimazine 2,3,6-Trichlorobenzoic acid
Use	Herbicide, plant growth regulator, phytocide. Interferes with plant production of histidine; reagent in photography. Use on food croplands has been cancelled by EPA. Currently used for control of woody plants, annual grasses and broadleaf weeds; perennial broadleaf weeds and grasses; cattails; poison ivy; and certain aquatic weeds in marshes and drainage ditches (Sax 1986).
State and appearance	Colourless crystals.
Molecular weight	84.08
Water solubility, mg/l	280000 25 °C > 100000 (MITI 1992)
Melting point, °C	151–154 (MITI 1992)
Log octanol/water coefficient, log Pow	-1.9 (MITI 1992)
Mobility	Translocation of amitrole through the soil occurs in sandy, low humus soil in cool, damp weather (or when the groundwater level is high). Mobility decreases with increasing clay and humus content of the soil (Sax 1986).
Other physico-chemical properties	When strongly heated emits highly toxic fumes. Sublimes undecomposed under reduced pressure. Soluble in water.
Total degradation in water	Persists in water more than 200 days. Acts as a weak base and forms salts with acids (aqueous solutions are neutral) (Sax 1986). Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Other information about degradation	Impact on biodegradation processes: approx. 50% inhibition of NH3 oxidation in Nitrosomonas at 70 mg/l (Hooper & Terry 1973).

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Other information about metabolism	Freshwater algae remove amitrole from water at pH 7.5 or above. Uptake of amitrole by Scenedesmus quadricauda was directly related to herbicide concentration and easily metabolized (Sax 1986).
Bioconcentration factor, fishes	< 0.3 6w, Cyprinus carpio, conc 2 mg/l < 3.1 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
LD50 values to mammals in oral exposure, mg/kg	1100 orl-rat (Lewis & Sweet 1984) 1100–2500 orl-rat (Ames et al. 1973) 25000 orl-male albino rat (Anon. 1976) 14700 orl-mus (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	> 10000 skn-rat (Martin 1968) 200 ipr-mus (Sweet 1987)
TDLo values to mammals in oral exposure, mg/kg	2600 orl-mus, 6-18d preg. 1935 orl-mus, 6-14d preg. effects on embryo or fetus 113000 orl-mus, tumorigenic 366 orl-mus, tumorigenic 4595 orl-rat, tumorigenic 3670 orl-rat, tumorigenic 122000 orl-rat, tumorigenic 105 orl-rat, tumorigenic (Sweet 1987) 0.7 orl-rat, 22d preg, teratogenic (Sax 1986)
TDLo values to mammals in non-oral exposure, mg/kg	4176 scu-mus, 6-14d preg. eff. on fertility, embryo or fetus (Sweet 1987)
Other information about mammals	In diet: rats fed 50 ppm for 68 weeks suffered no effect on growth or food intake but the male rats developed an enlarged thyroid after thirteen weeks ; rats fed 500 ppm for 17 weeks and returned to normal diet 2 weeks before sacrifice appeared to have normal thyroids (Verschueren 1983).
Carcinogenicity	Carcinogenic (McCann et al. 1975). Cancer-suspect agent (Verschueren 1983: Amitrol induced thyroid and liver tumours in both mice and rats following oral and/or subcutaneous administration. An increased incidence of liver-cell tumours in the trout has also been reported following oral administration, but this cannot be conclusive. Limited skin-painting studies in mice gave no evidence of skin carcinogenicity. A single, small, cohort study raised the suspicion that amitrole may be carcinogenic to man, but the findings cannot be regarded as conclusive (Sax 1986).
Mutagenicity	Mutagenicity in the Salmonella test: none: < 0.001 revertant colonies/nmol; < 70 revertant colonies at 5 mg/plate (McCann et al. 1975). Mutagen data: dnd, esc, 0.010 mmol/l; pic, esc, 15 g/l; otr, rat, emb, 80 mg/l; hma, mus, sat, 12 mg/kg; otr, ham, emb, 10 mg/l (Sax 1986).
Teratogenicity	20 to 40 mg injected into chick yolk sacs during 0 to 96 hours incubation periods produced abnormalities of the beak and occasionally bent tibias (Sax 1986).
LD50 values to birds in oral exposure, mg/kg	> 100 orl-Agelaius phoeniceus > 316 orl-Coturnix coturnix (Schafer et al. 1983)

Effects on plants	3 or 4 day old corn seedlings (Zea mays) treated with nutrient solution which contained 80 mg/l of amitrole produced chlorotic tissues (McWhorter 1963). Incubation of segments of Sesbania exaltata hypocotyls in 1% sucrose containing 2 ppm amitrole inhibited protein synthesis by 19% (Mann et al. 1965). ATA caused inhibition of root elongation, when applied to the mature leaves of rooted cuttings of Populus tremula in quantities of > 0.1 mg per plant (in a lanolin paste containing 0.5% ATA) or to the growth solution in concentrations from 0.00003 M. In both cases the response was delayed about 24 hours (Eliasson 1962).
LC50 values to crustaceans, mg/l	> 23 Daphnia magna (Kenaga 1979) 30 48hr, Daphnia magna 32 48hr, Cypridopsis vidua (Sanders 1970)
LC50 values to fishes, mg/l	> 50 Salmo gairdneri (Kenaga 1979) 100 48 hr (Sanders 1970) 100 48 hr Lepomis macrochirus (Edwards 1977) 2100 96 hr, Gambusia affinis (Johnson 1978) 325 48 hr, Oncorhynchus kisutch (Bond et al. 1960) > 500 48 hr, Oryzias latipes (MITI 1992)
Other information about water organisms	Crustacean: no effect level: Gammarus fasciatus; 100 mg/l, 48 hr no effect level: Asellus brevicaudus; 100 mg/l, 48 hr no effect level: Palaemonetes kadiakensis;100 mg/l; no effect level: Orconectes nais; 100 mg/l,48 hr 48hr Fish: no effect level: Lepomis macrochirus: 100 mg/l,48 hr (Sanders 1970).

136 • Ammonia

7664-41-7

Sumformula of the chemical	NH3
Use	Chemical industry, fertilizer
State and appearance	Colourless gas, liquified by compression.
Odour	Hedonic tone: extremely pungent. USSR: human odour perception: non perception: 0.4 mg/m³ perception: 0.5 mg/m³ human reflex response: no response: 0.22 mg/m³ adverse response: 0.35 mg/m³ animal chronic exposure: no effect: 0.2 mg/m³ adverse effect: 2.0 mg/m³ (Stern 1968).
Molecular weight	17.04
Specific gravity (water=1)	0.817 at 79 °C
Vapour density (air=1)	0.6
Conversion factor, 1 ppm in air=	0.707 mg/m³
Conversion factor, 1 mg/m³ in air=	1.414 ppm
Water solubility, mg/l	531000 at 20 °C
Melting point, °C	-77.7

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Boiling point, °C	-33.4	
Other physicochemical properties	In the neutral pH ammonia is in ionform and less toxic than ammonia (Nikunen et al. 1986)	
LD50 values to mammals in oral exposure, mg/kg	350	orl-rat (Lewis & Sweet 1984)
LCLo values to mammals in inhalation exposure, ppm	20	ihl-hmn (Lewis & Sweet 1984)
TCLo values to mammals in inhalation exposure, ppm	2000	4 hr, ihl-rat (Lewis & Sweet 1984)
Health effects	Man: lethal; > 1700 ppm severe toxic effect; 500 ppm, 1 min. symptoms of illness: 200 ppm unsatisfactory: > 100 ppm (Verschueren 1983).	
Effects on arthropods	LC50, Baetis rhodani: 2.2 mg/l, 0.42d 1.9 mg/l, 1d 1.6 mg/l, 2d 1.4 mg/l, 4d 1.11 mg/l, 6.25d LC50, Chironomus riparius: 3.2 mg/l, 0.42d 2.5 mg/l, 1d 1.75 mg/l, 2d 1.36 mg/l, 4d 1.14 mg/l, 6.25d (Williams et al. 1986).	
Effects on plants	Conifers were exposed to NH_3 for 50 days (in winter, open-top chambers): 0.42 mg NH_3/m^3 (95 perc.) - 0.25 mg NH_3/m^3 (mean) (0.61 ppm–0.36 ppm) caused heavy injury e.g. sharply bondered necrotic tip of the older needles of Taxus baccata. No-adverse-effect level for some months exposures: 0.2 mg/m³ (0.3 ppm). Eerden	
LC50 values to crustaceans, mg/l	5.02	96hr, Asellus racovitzai
	18.3	96hr, Orconectes immunis
	1.71	96hr, Simocephalus cetulus (Arthur et al. 1987)
	3.33	1d, Asellus aquaticus
	2.5	2d, Asellus aquaticus
	1.9	4d, Asellus aquaticus
	1.63	6.25d, Asellus aquaticus
	3.4	0.42d, Gammarus pulex
	2.6	1d, Gammarus pulex
	2.08	2d, Gammarus pulex
	1.69	4d, Gammarus pulex
	1.44	6.25d, Gammarus pulex (Williams et al. 1986)
	70	96hr, 21 °C, Nitocra spinipes (Linden et al. 1979)

LC50 values to fishes, mg/l	0.056	72 hr, Salmo gairdneri (Calamari et al. 1981)
	0.16–1.1	96 hr, Salmo gairdneri (Thurston & Russo 1983)
	0.75–3.4	96 hr, Pimephales promelas (Thurston et al. 1983)
	0.5–0.8	96 hr, Salmo clarci (Rubin & Elmaraghy 1977)
	> 3.58	fertilized egg, 24 hr, S.gairdneri
	> 3.58	alevins, 24 hr, S.gairdneri
	0.068	24hr, Salmo gairdneri, fry
	0.097	24hr, Salmo gairdneri (Rice & Stokes 1975)
	0.16–0.49	96hr, Salmo gairdneri (Calamari et al. 1981)
	2.17	96hr, Pimephales promelas
	0.53	96hr, Salmo gairdneri
	0.66	96hr, Stizostedion vitreum
	0.86	Ictalurus punctatus
	1.53	Catostomus commersoni (Arthur et al.1987)
	0.35	undissociated, as N, 16d Rutilus rutilus (Solbe et al. 1985)
LOEC values to fishes, mg/l	0.02	Salmo gairdneri (Thurston et al. 1984)
	0.64	phy, chr, Pimephales promelas (Smith 1984)
Other information about water organisms	Channa punctatus, 1–30 d, 30 mg/l, biochemical effect (Bjattacharya et al. 1987).	
Other effects on aquatic ecosystems	Impact on biodegradation processes: 2.0 mg/l affects the selfpurification of water courses (Verschueren 1983).	
Other information	Ammonium ion is less toxic then ammonia appearing at high pH-values.	

137 • Ammonium sulfate

7783-20-2

Synonyms	Diammonium sulfate Sulfuric acid, diammonium salt	
Sumformula of the chemical	04S.2H4N	
Use	Fertilizers; fermentation; viscose rayon; tanning; food additive.	
State and appearance	Brownish-gray to white crystals.	
Molecular weight	132.16	
Specific gravity (water=1)	1.77	
LD50 values to mammals in oral exposure, mg/kg	3000	orl-rat (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	610	ipr-mus (Sweet 1987)
LDLo values to mammals in oral exposure, mg/kg	3500	orl-domestic animal (Sweet 1987)
TDLo values to mammals in oral exposure, mg/kg	1500	orl-man, gastrointestinal changes (Sweet 1987)
LC50 values to crustaceans, mg/l	292	100 hr, Daphnia magna (Freeman 1953)
LC50 values to fishes, mg/l	310	96 hr, Alburnus alburnus (Linden et al. 1979)
	126	96 hr, Poecilia reticulata (Chouhan & Pandey 1987)
Effects on the physiology of water organisms	Channa punctatus: 21 mg/l, 180 days; histological effect (presence of physical damage to tissues) (Ram & Sathyanesan 1987).	

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138 • Ammonium sulfite 10196-04-0

Sumformula of the chemical	(NH4)2SO3H2O	
Use	Chemical intermediate; medicine; photography.	
State and appearance	Colourless crystals; acrid; sulfurous taste.	
Specific gravity (water=1)	1.41	
Sublimation point, °C	150	with decomposition
LC50 values to crustaceans, mg/l	203	100 hr, Daphnia magna (Freeman 1953)

139 • Ammoniumacetate 631-61-8

Sumformula of the chemical	CH3COONH4	
Use	Drugs; textile dyeing; foam rubbers; vinylplastics.	
Specific gravity (water=1)	1.07	
Melting point, °C	114	
LC50 values to fishes, mg/l	238	24 hr, Gambusia affinis (Jones 1971)
Effects on the physiology of water organisms	Tilapia mossambica; 0.001 M, 2 days; enzyme effect (change in enzyme activity) (Begum 1987).	

140 • Ammoniumcarbonate 506-87-6

LC50 values to fishes, mg/l	37	96 hr, Pimephales promelas (Curtis & Ward 1981)

141 • Ammoniumchloride 12125-02-9

Sumformula of the chemical	NH4Cl	
Use	Dry batteries; soldering; manufacture of various ammonia compounds fertilizer; electroplating.	
State and appearance	White crystals.	
Specific gravity (water=1)	1.54	
Sublimation point, °C	350	
LC50 values to crustaceans, mg/l	50	96 hr, Daphnia magna (Dowden & Bennet 1965)
	4.08	4d, as NH3, Asellus racovitzai
	4.19	4d, as NH3, Asellus racovitzai
	1.34	4d, as NH3, Crangonyx pseudogracilis
	4.64	4d, as NH3, Crangonyx pseudogracilis
	12.12	4d, as NH3, Orconectes immunis
	18.81	4d, as NH3, Orconectes immunis
	1.05	2d, as NH3, Simocephalus vetulus
	1.89	2d, as NH3, Simocephalus vetulus (Arthur et al. 1987)

LC50 values to fishes, mg/l	649	24 hr, Carassius carassius (Freeman 1953)
	1.83	4d, as NH3, Catostomus commersoni
	0.63	4d, as NH3, Catostomus commersoni
	1.06	4d, as NH3, Ictalurus punctatus
	0.41	4d, as NH3, Ictalurus punctatus
	2.1	4d, as NH3, Pimephales promelas
	1.51	4d, as NH3, Pimephales promelas
	0.86	4d, as NH3, Salmo gairdneri
	0.21	4d, as NH3, Salmo gairdneri
	0.9	4d, as NH3, Stizostedion vitreum vitreum
	0.42	4d, as NH3, Stizostedion vitreum vitreum (Arthur et al. 1987)
Effects on the physiology of water organisms	Cyprinus carpio; 0.400 mm/100 g, 0.01 d, haematological effect (change in various blood parameters such as red blood cell count, haematocrit, and serum osmolarity) (Ogata & Murai 1987). Ictalurus punctatus; 0.009 mg/l, 177 days, growth (measurable change in length and/or weight (Hermanutz et al. 1987). Pimephales promelas; 0.007 mg/l, 30 days, growth (measurable change in length and/or weight (Hermanutz et al. 1987). Salmo gairdneri; 0.009 mg/l, 237 days, growth (measurable change in length and/or weight (Hermanutz et al. 1987). Invertebrates; 0.016 mg/l, 90 days, population (change in number of species groups in a given community, that is, species diversity) (Hermanutz et al. 1987).	
Other information about water organisms	LC50, 96hr, 70 mg/l, Lymnea sp. (Dowden & Bennet 1965).	

142 • Ammoniumferricyanide 14221-48-8

LC50 values to fishes, mg/l	300	96 hr, Lepomis macrochirus (Dawson et al. 1977)

143 • Ammoniumfluoride 12125-01-8

Sumformula of the chemical	NH4F	
Use	Fluorides; antiseptic in brewing; wood preservation.	
State and appearance	White crystals.	
Specific gravity (water=1)	1.31	
LC50 values to crustaceans, mg/l	93	48 hr, Palaemonetes pugio (Curtis et al. 1979)
LC50 values to fishes, mg/l	364	96 hr, Pimephales promelas (Curtis et al. 1979)

144 • Ammoniumpicrate 131-74-8

Synonyms	Ammoniumcarbazotate Ammoniumpicronitrate	
Use	Explosive; medicine.	
State and appearance	Yellow crystals.	
Specific gravity (water=1)	1.72	
LC50 values to fishes, mg/l	220	96 hr, Lepomis macrochirus
	66	96 hr, Menidia audens (Dawson et al. 1977)

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145 • Amobarbital 57-43-2

LC50 values to fishes, mg/l	85.4	96hr, Pimephales promelas (Geiger et al. 1988)

146 • Amphetamine sulfate 60-13-9

LC50 values to fishes, mg/l	28.8	96hr, Pimephales promelas (Geiger et al. 1988)

147 • Amprolium 121-25-5

Synonyms	1-((4-Amino-2-propyl-5-pyrimidinyl)methyl)-2-picoliniumchloride	
Use	A coccidiostat.	
LC50 values to fishes, mg/l	270 1550	48hr, Poecilia reticulata (Canton & van Esch 1976) 48hr, Salmo gairdneri (Verschueren 1983)

148 • Amyl alcohol 71-41-0

Synonyms	1-Pentanol n-Pentyl alcohol	
Use	Solvent.	
Odour	Quality: sweet Hedonic tone: pleasant Threshold odour concentration: absolute: 0.12 ppm 50% recognition: 1.0 ppm 100% recognition: 1.0 ppm Odour index 100% recognition: 13 150 (Hellman & Small 1974).	
Molecular weight	88.15	
Water solubility, mg/l	26000	20 °C
Boiling point, °C	137.3	
Log octanol/water coefficient, log Pow	1.51	(Sangster 1989)
Volatilization	Relative volatility (nBuAc=1) = 0.23	
LD50 values to mammals in oral exposure, mg/kg	3030	orl-rat
Maximum longterm immission concentration in air for plants,mg/m³	20	VDI 2306
Maximum longterm immission concentration in air for plants,ppm	5	VDI 2306
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 220 mg/l (Bringmann & Kühn 1980a).	
EC50 values to microorganism, mg/l	5377	Biodegradation inhibition (Vaishnav 1986)
LOEC values to algae, mg/l	17	rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)

LC50 values to crustaceans, mg/l	440 96hr, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	530 96 hr, Branchydanio rerio (Wellens 1982) 479–492 48 hr, Leuciscus idus (Wellens 1982) 475 96 hr, Alburnus alburnus (Linden et al. 1979) 606 96hr, Pimephales promelas (Broderius & Kahl 1985)
Other information about water organisms	LOEC 17 mg/l, rpd, schr, Entosiphon sulcatum (Bringmann & Kühn 1980a). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 260 mg/l protozoa (Entosiphon sulcatum): 17 mg/l (Bringmann & Kühn 1980a).

149 • Amyl cinnamic aldehyde 122-40-7

Synonyms	Heptanal, 2-(phenylmethylene)-
Sumformula of the chemical	C14H180
EINECS-number	2045415
Water solubility, mg/l	100 (MITI 1992)
Boiling point, °C	285 (MITI 1992)
Total degradation in water	Biodegradation: 51% by BOD (on the upward trend) period: 28 d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

150 • n-Amylacetate 628-63-7

Synonyms	prim-Amylacetate 1-Pentanolacetate Amylacetic ester Amylacetate
Sumformula of the chemical	CH3COOC5H11
Use	Solvent.
Odour	Characteristic. Quality: sweet, ester, banana. Hedonic tone: pleasant. Odour index: 25.047 (Hellman & Small 1974). Threshold: unadapted panellists: 20 ppm after adaption with pure odourant: 3000 ppm (Verschueren 1983). Human odour perception: non perception: 0.5 mg/m^3 perception: 0.6 mg/m^3 = 0.11 ppm human reflex response: no response: 0.12 mg/m^3 adverse response: 0.30 mg/m^3 (Stern 1968).
Molecular weight	130.2
Specific gravity (water=1)	0.879 at 20/20 °C

Conversion factor, 1 ppm in air=	5.32	mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.188	ppm
Water solubility, mg/l	1800	at 20 °C
Boiling point, °C	148 149.3	at 737 mm
Volatilization	Relative volatility (nBuAc=1) = 0.42	
Other information about degradation	Impact on biodegradation processes: Inhibition by degradation of glucose by Pseudomonas fluorescens at 350 mg/l; inhibition of degradation of glucose by Escherichia coli at: > 1000 mg/l (Bringmann & Kühn 1960).	
LD50 values to mammals in oral exposure, mg/kg	7400	orl-rbt
Effects on microorganisms	Bacteria: Escherichia coli: no effect level; 1 g/l (Meinck et al. 1970). Toxicity threshold (cell multiplication inhibition test): bacteria: Pseudomonas putida: 145 mg/l (Bringmann & Kühn 1980a).	
LOEC values to algae, mg/l	63 80	rpd, act, Microcystis aeruginosa (Bringmann & Kühn 1976) rpd, act, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
LC50 values to fishes, mg/l	10 650 180	96 hr, Carassius auratus (Verschueren 1983) 96 hr, Lepomis macrochirus 96 hr, Menidia beryllina (Dawson et al. 1977)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): algae: Microcystis aeruginosa: 63 mg/l green algae: Scenedesmus quadricauda: 80 mg/l protozoa (Entosiphon sulcatum): 226 mg/l protozoa (Uronema parduczi): 550 mg/l (Bringmann & Kühn 1976, 1980a). Crustacean: Daphnia: 48 hr threshold toxic effect at 23 °C: 440 ppm (McKee & Wolf 1971).	

151 • Amylchloride 543-59-9

Synonyms	1-Chloropentane Pentylchloride	
Sumformula of the chemical	CH3(CH2)3CH2Cl	
Molecular weight	106.6	
Specific gravity (water=1)	0.883	at 20/4 °C
Vapour density (air=1)	3.67	
Melting point, °C	-99	
Boiling point, °C	108.2	
Henry's law constant, Pa x m^3/mol	4942	calc. (Yaws et al. 1991)

152 • Anilazine

101-05-3

Synonyms	2-Chloro-N-(4,6-dichloro-1,3,5-triazin-2-yl)aniline	
Use	Fungicide.	
LD50 values to birds in oral exposure, mg/kg	> 100	orl-Agelaius phoeniceus (Schafer et al. 1983)
LC50 values to crustaceans, mg/l	4.5	act, Daphnia pulex (Nishiuchi & Hashimoto 1967)
LC50 values to fishes, mg/l	0.095	48hr, Cyprinus carpio (Nishiuchi & Hashimoto 1967)

153 • Aniline

62-53-3

Synonyms	Phenylamine Aminobenzene Benzenamine		
Sumformula of the chemical	C6H7N		
Use	Intermediate.		
Odour	Characteristic. Hedonic tone: pungent. Human odour perception: non perception: 0.34 mg/m³; perception: 0.37 mg/m³ Human reflex response: adverse response: 0.07 mg/m³ Animal chronic exposure: adverse effect: 0.05 mg/m³ (Stern 1968).		
Molecular weight	93.14		
Specific gravity (water=1)	1.02		
Vapour density (air=1)	3.22		
Conversion factor, 1 ppm in air=	3.87	mg/m³	
Conversion factor, 1 mg/m³ in air=	0.259	ppm	
Vapour pressure, mmHg	1 0.3	35 °C 20 °C	
Water solubility, mg/l	34000		
Melting point, °C	-6		
Boiling point, °C	184		
Log octanol/water coefficient, log Pow	0.9 0.95 0.9	(Anon. 1986) (Anon. 1988) (Sangster 1989)	
Log soil sorption coefficient, log Kom	1.17	(Sabljic 1987)	
Henry's law constant, Pa x m³/mol	0.11	(Anon. 1988)	

Mobility	Equilibrium distribution: *mass %* air 3.64 water 96.23 solid 0.13 (Anon. 1988).
Photochemical degradation in water	Photo oxidation by ultra violet light in aqueous medium at 50 °C: 28.5% degradation to CO_2 after 24 hours (Knoevenagel & Himmelreich 1976).
Total degradation in soil	Decomposition period by a soil micro flora: 4 days (Verschueren 1983).
Other information about degradation	75% inhibition of nitrification in the activated sludge process at 7.7 mg/l degree of inhibition of NH_3 oxidation by Nitrosomonas sp.: at 100 mg/l, 86% inhibition at < 1 mg/l, approx. 50% inhibition (Hockenbury & Grady 1977).
LD50 values to mammals in oral exposure, mg/kg	250 orl-rat 195 orl-dog (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	254 skn-cat (Lewis & Sweet 1984)
LDLo values to mammals in non-oral exposure, mg/kg	820 skn-rbt 150 unk-man (Lewis & Sweet 1984)
Health effects	Man: severe toxic effects: 80 ppm, 60 min symptoms of illness: 20 ppm unsatisfactory: > 10 ppm (Verschueren 1983).
Mutagenicity	Mutagenicity in the Salmonella test: neg., < 0.005 revertant colonies/nmol; < 70 revertant colonies at 1 mg/plate (McCann et al. 1975).
LD50 values to birds in oral exposure, mg/kg	562 orl-Agelaius phoeniceus ≥ 1000 orl-Sturnus vulgaris 750 orl-Coturnix coturnix 562 orl-Passer domesticus (Schafer et al. 1983)
Effects on amphibia	Amphibian: lethality and teratogenicity to early embryonic stages of South African clawed frog, Xenopus laevis:

mg/l	day 1 A/S, %	day 2 A/S, %	day 3 A/S, %	day 4 A/S, %
0	0/50, 0	0/50, 0	0/50, 0	0/50, 0
10	0/50, 0	0/47, 0	4/36, 11	4/36, 11
50	1/50, 2	3/48, 6	3/48, 6	3/48, 6

(A/S = abnormals/survivors) (Dumont et al. 1979).

Mexican axolotl (3–4 weeks after hatching):48 hr LC50:440 mg/l
Clawed toad (3–4 weeks after hatching): 48 hr LC50: 560 mg/l
(Slooff & Baerselman 1980).

Effects on arthropods	Tanytarsus dissimilis: LC59, 2 days, > 219 mg/l (Holcombe et al. 1987).
Maximum longterm immission concentration in air for plants, mg/m³	0.24 VDI 2306

Maximum longterm immission concentration in air for plants, ppm	0.2	VDI 2306
Effects on microorganisms		Bacteria: Escherichia coli: no effect at 1 g/l (Bringmann & Kühn 1976). Toxicity threshold (cell multiplication inhibition test): bacteria: Pseudomonas putida: 130 mg/l (Bringmann & Kühn 1980).
Effects on wastewater treatment		Degradation by Aerobacter: 500 mg/l at 30 °C: parent: 100% ring disruption in 54 hours mutant: 100% ring disruption in 12 hours (Verschueren 1983).
EC50 values to algae, mg/l	19	96hr, rpd, Selenastrum capricornutum (Calamari et al. 1982)
LOEC values to algae, mg/l	0.16	Microcystis aeruginosa (Bringmann & Kühn 1976)
	8.3	rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
NOEC values to algae, mg/l	10	rpd, schr, Selenastrum capricornutum (Slooff et al. 1983)
LC50 values to crustaceans, mg/l	0.55	48 hr, Daphnia magna
	0.1	48hr, Daphnia pulex
	0.68	48hr, Daphnia cucullata (Canton & Adema 1978)
	68	48hr, Asellus aquaticus (Slooff 1983)
	112	48hr, Gammarus pulex (Slooff 1983)
EC50 values to crustaceans, mg/l	0.66	14d, rpd, Daphnia magna (Hattori et al. 1984)
	0.25	2d, Daphnia magna (Holcombe et al. 1987)
LC50 values to fishes, mg/l	20	96 hr, Salmo gairdneri (Calamari et al. 1980)
	8.2	7 d, Salmo gairdneri (Abram & Sims 1982)
	32–33	96 hr, Branchydanio rerio
	61–78	48 hr, Leuciscus idus (Wellens 1982)
	43	48 hr, Salmo gairdneri (Slooff et al.1983)
	36.3	act, Salmo gairdneri (Hodson et al. 1984)
	187	4d, Carassius auratus
	78.4	4d, Catostomus commersoni
	49	4d, Lepomis macrochirus
	40.5	4d, Salmo gairdneri
	77.9	4d, Pimephales promelas (Holcombe et al. 1987)
Effects on the physiology of water organisms		Inhibition of photosynthesis of a fresh water non-axenic uni-algal culture of Selenastrum capricornutum: at 10 mg/l: 90% carbon-14 fixation (vs controls) at 100 mg/l: 34% carbon-14 fixation (vs controls) at 1000 mg/l: 3% carbon-14 fixation (vs controls) (Verschueren 1983). Aquatic community; 4 days, 1–300 mg/l; stress effect (observed physiological tension in animals or plants) (Yount & Shannon 1987).

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Other information about water organisms	EC50, 24hr, 190 mg/l, rpd, Tetrahymena pyriformis (Yoshioka et al. 1985). Protozoa: ciliate (Tetrahymena pyriformis): 24 hr LC100: 21.5 m mole/l (Schultz et al. 1978). Algae: Scenedesmus: toxic: 10 mg/l Microcystis aeruginosa: inhibition of cell multiplication starts at 0.16 mg/l; LD50 20 ppm (Bringmann & Kühn 1976; Verschueren 1983). Arthropoda: Daphnia: toxic: 0.4 mg/l (Bringmann & Kühn 1980). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 8.3 mg/l protozoa (Entosiphon sulcatum): 24 mg/l protozoa (Uronema parduczi): 91 mg/l (Bringmann & Kühn 1980). Aplexa hypnorum; LC50, 4 days, > 219 mg/l (Holcombe et al. 1987). LC50, 48hr, 450 mg/l, Tubificidae LC50, 48hr, 175 mg/l, Chironomus gr. thummi LC50, 48hr, 760 mg/l, Erpobdella octoculata LC50, 48hr, 800 mg/l, Lymnaea stagnalis LC50, 48hr, 155 mg/l, Dugesia cf. lugubris LC50, 48hr, 406 mg/l, Hydra oligactis LC50, 48hr, 150 mg/l, Corixa punctata LC50, 48hr, 235 mg/l, Ischura elegans LC50, 48hr, 64 mg/l, Nemoura cinerea LC50, 48hr, 220 mg/l, Cloeon dipterum (Slooff 1983).

154 • Aniline hydrochloride 142-04-1

Synonyms	Anilinechloride Aniline chloride, aniline salt Hydrochloride benzenamide Phenylamine–hydrochloride
Sumformula of the chemical	C6H7N.ClH
Use	Dye intermediate; dyeing and printing.
State and appearance	White crystals, darkens in light and air.
Molecular weight	129.59
Specific gravity (water=1)	1.2215
Vapour density (air=1)	4.46
Melting point, °C	198
Boiling point, °C	245
Flashing point, °C	193
Other physicochemical properties	Slight fire hazard when exposed to flame or hear; emits toxic aniline and chlorine fumes when decomposed or reacted with acid. Soluble in alcohol, ether. Soluble in approximately 1 part water.

Metabolism in mammals	Administration of 50 mg/kg injected ivn to rabbits had a half–life in the blood of 295 min (n=6). – When added to the perfusion fluid in amounts of 0.0002–0.100 mmol aniline hydrochloride was poorly accumulated (10–20%) by isolated perfused rabbit lungs, artificially ventilated and perfused via the pulmonary artery with heparin treated, antologous whole blood. Uptake was rapid and steady-state was reached in 10 minutes. – Male rats were administered aniline HCl by gavage at 3 doses: 10, 30, and 100 mg/kg. At selected times, rats were sacrificed and brain, lung, kidney, liver, spleen, heart and plasma analyzed for radioactivity. Urine and feces were collected at 12 hr intervals for 48 hr after treatment. Results: Peak plasma radioactivity was observed at 0.5, 1.0, and 2.0 hr for 10, 30, and 100 mg/kg doses, respectively. By 24 hr after dosing, the plasma radioactivity had decreased to < 2 % of peak concentration for all dosages. Radioactivity was distributed to all tissues, with highest peak levels observed in the kidney, followed by liver, plasma, lung, heart, spleen and brain for all doses. By 48 hr after dosing, < 0.1% of total administered radioactivity at any of the three doses remained in any of the tissues examined. Recovery of radioactivity in urine 48 hr after dosing was 96, 91, and 77% for the 10, 30, and 100 mg doses, respectively. Results indicate that aniline HCl is rapidly eliminated from the rat in the urine, particularly as an acid-hydrolyzable metabolite of p-aminophenol. – The gastrointestinal tract seems to be a major site for the metabolism of aniline in the rat following ivn injection of 3, 30 or 100 mg/kg to male Fischer 344 rats (Sax 1986).
LD50 values to mammals in oral exposure, mg/kg	1072 orl-rat) 841 orl-mus (Sax 1986
LD50 values to mammals in non-oral exposure, mg/kg	300 ipr-mus (Sax 1986)
LDLo values to mammals in non-oral exposure, mg/kg	500 ipr-rat (Sax 1986)
TDLo values to mammals in oral exposure, mg/kg	130000 orl-rat, 2Y-C, tumorigenic (Sax 1986)
Health effects	Skin and eye irritation data: skn, rbt, 500 mg, 24 hr, moderate; eye, rbt, 20 mg, 24 hr, severe (Sax 1986).
Carcinogenicity	Dietary administration was found to be carcinogenic to male and female Fischer 344 rats, inducing hemangiosarcomas and a combination of fibrosarcomas and sarcomas, NOS or the spleen and a combination of fibrosarcomas and sarcomas, NOS of multiple body organs. There was no evidence of carcinogenicity in mice of either sex (Sax 1986).
Mutagenicity	Mutagen data: otr, rat, emb, 79500 ng/plate; sce, ham, fbr, 0.010 mmol/L (Sax 1986). NCI carcinogenesis bioassay completed; result positive: rat; results negative: mouse (Sax 1986).
LC50 values to fishes, mg/l	5.5 48 hr, Carassius auratus (McKee & Wolf 1963)
Other information about water organisms	Fish: goldfish, approx. fatal conc. 5.5 mg/l, 48hr (McKee & Wolf 1963). *effect level (mg/l)* Chironomus dorsalis 7.8 Chironomus dorsalis 5.0 Carassius auratus 5.5 (48 hr) Cyprinus carpio 0.5–48.0 (90 days) Cyprinus carpio 0.1 (90 days) (Sax 1986).

155 • m-Anilinesulfonic acid 121-47-1

Total degradation in soil	Decomposition period by a soil micro flora: > 64 days (Verschueren 1983).

156 • o-Anilinesulfonic acid 88-21-1

Total degradation in soil	Decomposition period by a soil micro flora: > 64 days (Verschueren 1983).

157 • p-Anilinesulfonic acid 121-57-3

Synonyms	Sulfanilic acid p-Aminobenzenesulfonic acid
State and appearance	Colourless crystals.
Molecular weight	191.2
Water solubility, mg/l	10800 at 20 °C 66700 at 100 °C
Degradation point, °C	288
Total degradation in soil	Decomposition by a soil micro flora in > 64 days (Verschueren 1983).
LD50 values to mammals in oral exposure, mg/kg	> 3200 orl-mus (Patty 1967)
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

158 • m-Anisic acid 586-38-9

Synonyms	3-Methoxybenzoic acid
State and appearance	Colourless needles.
Molecular weight	152.14
Melting point, °C	107–110
Boiling point, °C	170–172 °C, at 10 mmHg
Log octanol/water coefficient, log Pow	2.02
Total degradation in soil	Decomposition period by a soil microflora: 16 days (Verschueren 1983).

159 • o-Anisic acid 579-75-9

Synonyms	2-Methoxybenzoic acid Salicylic acid methylether
Molecular weight	152.14
Specific gravity (water=1)	1.18
Water solubility, mg/l	5000 at 30 °C
Melting point, °C	101
Boiling point, °C	200
Total degradation in soil	Decomposition period by a soil micro flora: 4 days (Verschueren 1983).

160 • p-Anisic acid

100-09-4

Synonyms	4-Methoxybenzoic acid	
Molecular weight	152.14	
Specific gravity (water=1)	1.385	at 4/4 °C
Water solubility, mg/l	400	at 18 °C
Melting point, °C	275–280	
Log octanol/water coefficient, log Pow	1.96	
Total degradation in soil	Decomposition period by a soil microflora: 2 days (Verschueren 1983).	

161 • m-Anisidine

536-90-3

Synonyms	3-Methoxyaniline 3-Aminoanisole	
Molecular weight	123.15	
Specific gravity (water=1)	1.096	at 20/4 °C
Melting point, °C	< - 12 °C	
Boiling point, °C	251	
Log octanol/water coefficient, log Pow	0.93	
Total degradation in soil	Decomposition period by a soil micro flora: > 64 days (Verschueren 1983).	
LD50 values to birds in oral exposure, mg/kg	562 > 1000 562	orl-Agelaius phoeniceus orl-Sturnus vulgaris orl-Coturnix coturnix (Schafer et al. 1983)
Effects on wastewater treatment	Degradation by Aerobacter: ring disruption:	500 mg/l at 30 °C: parent: 80% in 120 hours mutant: 100% in 24 hours (Verschueren 1983).

162 • Anisole

100-66-3

Synonyms	Phenol methyl ether	
Sumformula of the chemical	C7H8O	
Water solubility, mg/l	100	(MITI 1992)
Melting point, °C	-37	(MITI 1992)
Boiling point, °C	155–156	(MITI 1992)
Log octanol/water coefficient, log Pow	2.1 2.11	(Anon. 1986) (Sangster 1989)
Log soil sorption coefficient, log Kom	1.3	(Sabljic 1987)

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Total degradation in water	Biodegradation: 56% by BOD (on the upward trend) period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

163 • Anthracene

120-12-7

Sumformula of the chemical	$C_{14}H_{10}$	
Use	Dyes.	
Molecular weight	178.23	
Specific gravity (water=1)	1.25	
Vapour density (air=1)	6.15	
Water solubility, mg/l	1.29 0.6 < 1	at 25 °C in distilled water at 25 °C in salt water (MITI 1992)
Melting point, °C	217	(MITI 1992)
Boiling point, °C	339.9	(MITI 1992)
Log octanol/water coefficient, log Pow	4.54 4.33 4.34 4.5	(Chin et al. 1986) (Chin et al. 1986) (Mackay 1982) (Sangster 1989)
Adsorption/desorption	Adsorption on smectite clay particles from simulated seawater at 25 °C – experimental conditions: 0.1 mg anthracene/l; 50 mg smectite/l-adsorption: 0.0009 mg/mg = 46% adsorbed (Meyers & Oas 1978).	
Other bindings	After 3 hr incubation in natural seawater, 11% of 0.015 mg/l were taken up by suspended aggregates of dead phytoplankton cells and bacteria (Verschueren 1983).	
Total degradation in water	Biodegradation: 1.9% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992)	
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).	
Other information about metabolism	Daphnia pulex: Excretion of 14C - after 16 hr incubation with 14C-anthracene and subsequent transfer to clean water resulted in a rapid release (1 hr) of about 30% of the total 14C, a more slow elimination of roughly 60% with a half-life of 3.3 hr and a tightly bound residue of 8%. The observed rate of metabolite excretion during the first 24 hr of excretion was only 6% of the total 14C outflux rate (Herbes & Risi 1978).	
Bioconcentration factor, fishes	1660–2820 903–2710	8w, Cyprinus carpio, conc 0.015 mg/l 8w, Cyprinus carpio, conc 0.0015 mg/l (MITI 1992)
Bioconcentration factor, mollusca	430 2500	2 days, oysters/water 8 days, oysters/water (Lee et al. 1978)

Bioconcentration factor, crustaceans	760 Daphnia pulex (Herbes & Risi 1978)
Other information about bioaccumulation	Confirmed to be accumulated on a medium level (Anon. 1987).
Carcinogenicity	Carcinogenicity: negative (Verschueren 1983).
Mutagenicity	Mutagenicity in the Salmonella test: negative; < 0.01 revertant colonies/n mol < 70 revertant colonies at 1 mg/plate (Verschueren 1983).
LD50 values to birds in oral exposure, mg/kg	> 111 orl-Agelaius phoeniceus > 244 orl-Passer domesticus (Schafer et al. 1983)
Effects on arthropods	LC50, 1 day; < 0.001 mg/l, Aades aegypti LC50, 1 day; 0.260 mg/l, Aades taeniorhynchus LC50, 1 day; 0.037 mg/l, Culex quinquefasciatus (Borovsky et al. 1987).
LC50 values to fishes, mg/l	> 210 48hr, Oryzias latipes (MITI 1992)
NOEC values to fishes, mg/l	5 srv, act, 24 hr, Salmo trutta (Meinck et al. 1970)
Other information about water organisms	Algae: inhibition of photosynthesis of a freshwater, non axenic uni-algal culture of Selenastrum capricornutum at: 1% saturation: 99% carbon-14 fixation (vs. controls) 10% saturation: 104% carbon-14 fixation (vs. controls) 100% saturation: 99% carbon-14 fixation (vs. controls) (Verschueren 1983). Fish: trout; no effect level: 5 mg/l, 24hr (Meinck et al. 1970). Lethal threshold concentration (LT50): Daphnia magna; 0.015 mg/l 0.21 days (Newsted & Giesy 1987). Lethal threshold concentration (LT50): Pimephales promelas; 0.0054 mg/l, 0.66 days (Oris et al. 1987).

164 • Anthraquinone 84-65-1

Synonyms	9,10-Dihydro-9,10-diketoanthracene
Use	Intermediate for dyes and organics, bird repellent for seeds.
State and appearance	Yellow green crystals.
Molecular weight	208.2
Specific gravity (water=1)	1.419 at 20/4 °C
Melting point, °C	286 (MITI 1992)
Boiling point, °C	379–381 (MITI 1992)
Sublimation point, °C	286
Total degradation in water	Biodegradation: 52.3% by BOD (on the upward trend) period: 21d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

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Other information about degradation	Impact on biodegradation processes: at 2.5 mg/l inhibition of the selfpuration activity of natural waters (Meinck et al. 1970).
LD50 values to mammals in oral exposure, mg/kg	> 5000 orl-mus (Martin 1968)
LD50 values to birds in oral exposure, mg/kg	100–300 orl-Agelaius phoeniceus ≥ 100 orl-Passer domesticus (Schafer et al. 1983)
Other information about water organisms	Inhibition of photosynthesis of a freshwater non-axenic uni-algal culture of Selenastrum capricornutum: at 1% saturation: 97% carbon-14 fixation (vs. controls) at 10% saturation: 91% carbon-14 fixation (vs. controls) at 100% saturation: 85% carbon-14 fixation (vs. controls) (Verschueren 1983). Pimephales promelas, mortality, 96 hr, 0.240 mg/l (Geiger et al. 1988).

165 • Anthraquinone-α-sulfonic acid 65894-78-2

Synonyms	9,10-Dihydro-4-amino-4-benzoyl-9,10-dioxo-2-anthracenesulfonic acid
LC50 values to crustaceans, mg/l	50 96 hr, Daphnia magna (Dowden & Bennet 1965) 12 100 hr, Daphnia magna (Freeman 1953)

166 • Antimony and antimony compounds 7440-36-0

LC50 values to crustaceans, mg/l	> 530 48 hr, Daphnia magna (LeBlanc 1980)
LC50 values to fishes, mg/l	0.66 28 d, Salmo gairdneri (Birge et al. 1980)

167 • Antimycin 518-75-2

LC50 values to fishes, mg/l	0.0006 96 hr, Cyprinus carpio (Marking & Bills 1981)

168 • Antimycin A 1397-94-0

Use	Poison for Streptomyces aureus.
Molecular weight	548.7
LD50 values to mammals in oral exposure, mg/kg	28 orl-rat 1.8 orl-gpg (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	2 orl-pgn 2.9 orl-dck (Lewis & Sweet 1984)
LC50 values to fishes, mg/l	0.00009 96hr, Anguilla rostrata (Hinton & Eversole 1978) 0.003 96hr, Anguilla rostrata (Hinton & Eversole 1980) 0.00055 96hr, Esox lucius 0.00003 96hr, Salmo gairdneri (Kemp et al. 1973)

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169 • Aphidon
5827-05-4

Use	Insecticide.	
LC50 values to crustaceans, mg/l	0.01	act, Daphnia pulex (Nishiuchi & Hashimoto 1967)
LC50 values to fishes, mg/l	20	48hr, Cyprinus carpio (Pesticide Manual 1983)

170 • Aquaciene 100
53763-47-6

Use	Oil dispersant.	
LC50 values to fish, mg/kg	25	96hr, Pimephales promelas (Kemp et al. 1973)

171 • Aramite
140-57-8

Synonyms	2-(p-Butylphenox)isopropyl-2-chloroethylsulfite	
LD50 values to birds in oral exposure, mg/kg	> 100	orl-Agelaius phoeniceus (Schafer et al. 1983)
EC50 values to crustaceans, mg/l	0.18 0.16	48hr, mbt, Simocephalus serrulatus 48hr, mbt, Daphnia pulex (Sanders & Cope 1966)

172 • Arsenetrisulfide
1303-33-9

Synonyms	Arsenic trisulfide	
Sumformula of the chemical	As2S2	
Use	Pigment, reducing agent, pyrotechnics, glass used for infrared lenses, semiconductors, hair removal from hides.	
State and appearance	Yellow crystals or powder.	
Melting point, °C	300	
Other physicochemical properties	Insoluble in water and hydrochloric acid, dissolves in alkaline sulfide solutions and nitric acid.	
EC50 values to fishes, mg/l	135.1	srv, 96 hr, Pimephales promelas (Curtis et al. 1979)

173 • Arsenic acid
7778-39-4

Synonyms	Orthoarsenic acid	
Sumformula of the chemical	H3As04 . 1/2H20	
Use	Manufacture of arsenates, glass making, wood treating process, defoliant (regulated), desiccant for cotton, soil sterilant.	
State and appearance	White, translucent crystals.	
Melting point, °C	35.5	
Boiling point, °C	160	loses water at 160 °C
Other physicochemical properties	Soluble in water, alcohol, alkali, glycerol.	

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LC50 values to crustaceans, mg/l	2.1 6.6	2d, Daphnia magna 2d, Daphnia magna (Burton et al. 1987)

174 • Arsenic acid, disodium salt, heptahydrate 10048-95-0

Effects on the physiology of water organisms	Salmo gairdneri, 56 d, 0.120 mg/g, growth effect (Cockell & Hilton 1988).

175 • Arsenic acid, sodium salt 7631-89-2

Synonyms	Sodium arsenate	
Molecular weight	302.88	
Bioconcentration factor, algae	10000	arsenate, blue-green algae, dry weight Baltic sea (Blanck et al. 1989)
Effects on plants	Uptake of arsenate in plants is dependent on phosphate concentration (Blanck et al. 1989).	
LC50 values to algae, mg/l	 0.005-0.008 mg As/l	Arsenate: Fucus vesiculosus southern Baltic sea (Notini et al. 1987)
EC50 values to algae, mg/l	 0.006	Arsenate: As, periphyton, southern Baltic sea, pht (Blanck et al. 1989)
LOEC values to algae, mg/l	 0.0007–0.008 mg As/l 0.0002–0.0018 mg As/l 0.023	Arsenate phytoplankton, oligotrophic lake, pht periphyton, oligotrophic lake, pht (Wängberg 1989) as As, arsenate, periphyton, Skagerak, pht (Blanck et al. 1989)
LC50 values to fishes, mg/l	100	as As, arsenate, 48hr, Lepomis (Sorensen 1976)
Other information about water organisms	LOEC, 0.02 mg As/l, arsenate, Pontoporeia, reproduction, Baltic sea; LOEC, 0.023–0.075 mg As/l, Capitella, egg production, Skagerak (Blanck et al. 1989).	

176 • Arsenic and arsenic compounds 7440-38-2

Sumformula of the chemical	As
Molecular weight	74.92
Mobility	In well aerated top layer of water As is in the form of arsenate (80%), arsenite (10%), and mono and dimethylated acids (Blanck et al. 1989). In the Baltic sea there is a tendency of higher fraction of methylated forms (Andreae & Frowlich 1984). In sediment and in soil arsenate forms poorly soluble complexes with calcium, iron, sulfur etc. (Lemmo et al. 1983).
Other information about degradation	Degradation products of special interest: arsenic sugar (in algae); arsenocholine, arsenobetaine (in fish); trimethylarsinocide; trimethylarsine (Blanck et al. 1989).

Other information about metabolism	Water soluble, inorganic arsenic compounds are absorbed quickly through lungs, and gastrointestinal tract. Organic arsenic compounds (in fish) are absorbed effectively through gastrointestinal tract. 70% of arsenic in fish is eliminated in one year, the rest considerably slower (Vahter 1983).	
Bioconcentration factor, other organisms	100–200	invertebrates in fresh water (Fowler 1983)
Other information about bioaccumulation	There is a great variation with bioaccumulation between different arsenic compounds, plant and animal groups and species (Fowler 1983). Effective uptake of arsenocholine by fish by birth (40% retention). Most of arsenocholine (89%) accumulates as arsenobetaine (Francesconi et al. 1989).	
LDLo values to mammals in non-oral exposure, mg/kg	10 20 300	ipr-gpg ims-rat (Lewis & Sweet 1984) scu-gpg, scu-rbt (Sweet 1987)
TDLo values to mammals in oral exposure, mg/kg	7857 0.605 0.58 76	55 yr, orl-man (Lewis & Sweet 1984) orl-rat, 35 w preg., effects on fertility orl-rat, 30 pre/1-20d preg specific developmental abnormalities orl-man, 12 yr, tumorigenic (Sweet 1987)
TDLo values to mammals in non-oral exposure, mg/kg	75	implant-rbt, tumorigenic (Sweet 1987)
Carcinogenicity	Is not a direct mutagen but can injure DNA and inhibit DNA enzymes. In animal tests As functions probably as co-carcinogen (Squibb & Fowler 1983).	
Effects on amphibia	LD50, 96hr, 0.269 mg/l, tadpoles of Rana hexadactyla, Khangarot et al. 1985.	
LC50 values to crustaceans, mg/l	2.85 7.4	21 d, Daphnia magna 48 hr, without food, D. magna (Biesinger & Christensen 1972)
EC50 values to crustaceans, mg/l	1.4	21d, rpd, Daphnia magna (Biesinger & Christensen 1972)
LOEC values to crustaceans, mg/l	0.52	21d, rpd, Daphnia magna (Biesinger & Christensen 1972)
LC50 values to fishes, mg/l	30.5 40.5 0.55	96 hr, sft, Morone saxatilis 96 hr, hrd (Palawski et al. 1985) 24d, Salmo gairdneri (Birge et al. 1980)
LOEC values to fishes, mg/l	20	grw, phy, schr, Salmo gairdneri (Oladimeji et al. 1984)
NOEC values to fishes, mg/l	10	grw, phy, schr, Salmo gairdneri (Oladimeji et al. 1984)
Other information about water organisms	LC50, 48hr, 24.5 mg/l, Aplexa hypnorum (Holcombe et al. 1983).	

177 • Arsenic pentoxide 1303-28-2

Synonyms	Arsenic oxide Arsenic anhydride
Sumformula of the chemical	As205
Use	Arsenates, insecticides, dyeing and printing, weed killer, coloured glass, metal adhesive.
State and appearance	White amorphous solid, deliquescent.

Molecular weight	229.84	
Melting point, °C	315	
Other physicochemical properties	Forms arsenic acid in water. Soluble in water, alcohol.	
LD50 values to mammals in oral exposure, mg/kg	8 55	orl-rat orl-mus (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	330	ipr-rat (Lewis & Sweet 1984)

178 • Arsenic trioxide 1327-53-3

Synonyms	Arsenious acid Arsenious oxide Arsenious anhydride	
Sumformula of the chemical	As2O3	
Use	Pigments, ceramic enamels, aniline colours, decolorizing agent in glass, insecticide, rodenticide, herbicide, sheep and cattle dip, hide preservative, wood preservative, preparation of other arsenic compounds.	
State and appearance	White powder.	
Odour	Odourless, tasteless.	
Molecular weight	197.84	
Other physicochemical properties	Slightly soluble in water, soluble in acids and alkalies, soluble in glycerol.	
LD50 values to mammals in oral exposure, mg/kg	1.43 15.1 39.4	orl-man orl-rat orl-mus (Lewis & Sweet 1984)
LDLo values to mammals in oral exposure, mg/kg	10	orl-dog (Lewis & Sweet 1984)
Other information about mammals	LDfr = 100 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).	
Carcinogenicity	Human carcinogen (Sax & Lewis 1987)	
LD50 values to birds in oral exposure, mg/kg	13	orl-ckn (Lewis & Sweet 1984
Other information about birds	LDLo 13 mg/kg, idr-ckn (Lewis & Sweet 1984) LDLo 100 mg/kg, idr-pgn (Lewis & Sweet 1984)	
Effects on arthropods	LC50, 97.00 mg/l, 48hr, static, Tanytarsys dissimilis (Holcombe et al. 1983)	
LC50 values to crustaceans, mg/l	1	As, 7d, Daphnia magna (Spehar et al. 1980)
LC50 values to fishes, mg/l	17 14.7 10.9 10.9 18	96 hr, Coregonus sp. (Passino & Kramer 1980) 2d, Channa punctatus 4d, Channa punctatus (Burton et al. 1987) 4d, Channa punctatus (Shukla et al. 1987) 48hr, Puntius (Pandey & Shukla 1979)

Effects on the physiology of water organisms	Channa punctatus; 5 mg/l, 13 days: growth effect (measurable change in length and/or weight) (Burton et al. 1987). Salmo gairdneri, 56 d, 200 μg/g, growth effect (Cockell & Hilton 1988).
Other information about water organisms	LC50, 24.50 mg/l, 96hr, static, Aplexa hypnorum (Holcombe et al. 1983).
Other information	Use of As2O3, worldwide: wood preservative 16000 t/yr; dehydratant for cotton 12000 t/yr; herbicide 8000 t/yr; raw material in medicines 5000 t/yr; glass manufacturing 4000 t/yr; metal alloys, chemicals in industry 5000 t/yr 50000 t/yr (Chilvers & Peterson 1987).

179 • Asparagine

70-47-3

Synonyms	l-Asparagine 2-Aminobutanedioic amide l-α-Amino-succinamic acid l-β-Asparagine
Sumformula of the chemical	NH2COCH2CH(NH2)COOH
Use	Biochemical research; preparation of culture media; medicine.
Molecular weight	132.13
Specific gravity (water=1)	1.543 at 15/4 °C
Water solubility, mg/l	24600 at 25 °C 866000 at 100 °C
Degradation point, °C	235–236 °C
Other information	Natural sources; widely distributed in plants and animals, both free and combined with proteins.

180 • Aspartic acid

56-84-8

Synonyms	dl-Aspartic acid 2-Aminobutanedioic acid dl-Aminosuccinic acid Asparacemic acid
Sumformula of the chemical	COOHCH2CH(NH2)COOH
Use	Biochemical and clinical studies.
Molecular weight	133.1
Specific gravity (water=1)	1.663 at 12/12 °C
Water solubilitymg/l	8200 at 25 °C 47900 at 75 °C
Degradation point, °C	278–280
Other information	Natural source: a naturally occurring nonessential amino acid in young sugarcane and sugarbeet molasses.

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181 • Asulam

3337-71-1 * acid
2302-17-2 * Na-

Synonyms	Methyl sulfaninylcarbamate Methyl 4-aminobenzenesulfonylcarbamate (CAS 2302-17-2 * Na-)
Active ingredients	Methyl((4-aminophenyl)sulfonyl)carbamate * as Na salt; * 40% w/v
Use	Herbicide.
State and appearance	Colourless crystals.
Melting point, °C	143–144
Other information about degradation	Impact on biodegradation processes: Cellulose decomposition, measured as weight loss of buried cotton cloth, was reduced by 8–38% in treated soil at 16 ppm, after incubation at 19 °C for 8 weeks and by 0–60% in treated soil at 160 ppm. Experiments using pure cultures of soil-inhabiting fungi and actinomycetes, some of which were cellulolytic, showed that asulam at 10 ppm had either no, or only a temporary, effect on growth (Wingfield 1980).
LD50 values to mammals in oral exposure, mg/kg	> 5000 orl-rat, potassium salt 5000 orl-mus, potassium salt > 2000 orl-rbt, potassium salt > 1000 orl-ckn, potassium salt (Anon. 1976, Martin 1968)
Effects on plants	The seedlings of celery (Apium graveolens L.), whether germinated directly in asulam or transferred to an asulam solution containing 6 μmol asulam/l —inhibition of growth (Watts & Collin 1979).
LC50 values to fishes, mg/l	> 5000 96hr, Salmo gairdneri Ictalurus punctatus Carassius auratus > 3000 Lepomis macrochirus (Ingham & Gallo 1975) 5200 24hr, Rasbora heteromorpha (Alabaster 1969)

182 • Atrazine

1912-24-9

Synonyms	2-Ethylamino-6-isopropylamino-4-chloro-1,3,5-triazine 2-Chloro-4-ethylamino-6-isopropylamino-s-triazine
Sumformula of the chemical	C8H14ClN5
Use	Active ingredient in herbicides. Most widely used chemical for pre-emergence weed control in corn. In Hawaii it is important to the culture of sugarcane, pineapple, and macadamia nut.
State and appearance	Colourless crystals.
Molecular weight	215.72
Vapour pressure, mmHg	0.0000003 20 °C
Water solubility, mg/l	70 25 °C 33–45 20 °C
Melting point, °C	173–175
pKa	1.68
Log octanol/water coefficient, log Pow	2.6 (Anon. 1986) 2.68 (Anon. 1988) 2.64 (Anon. 1989) 2.63 (Mackay 1982)

Henry's law constant, Pa x m³/mol	0.00029 (Anon. 1988)
Mobility	Equilibrium distribution: *mass %* air 0.01 water 93.15 solid 6.84 (Anon. 1988). Theoretical distribution: sediment and soil 32%; water 68% (Nordic 1988).
Photochemical degradation in water	Photochemical degradation in UV-light (254 nm): in water solution Cl is changed with OH group (Esser et al. 1975).
Hydrolysis in water	Hydrolysis, pH 5, half-life: 64 d; pH 7–9, half-life > 200 d (Burkhard & Guth 1981).
Other chemical degradation processes	Hydrolysis: Cl breaks away , hydroxy derivatives are formed in sterile soil (Esser et al. 1975).
Half-life in soil, days	60 (Li et al. 1990) 96–204 (Dawson et al. 1980)
Total degradation in soil	75–100% disappearance from soils in 10 months (Verschueren 1983). In submerged soils: in 90 days 0.005% of atrazine-14C was recovered as 14CO2 (from ring labeled atrizine). 48% to 85% of atrazine was hydrolyzed in 30 days depending upon soil type. Chemical hydrolysis of atrazine to hydroxyatrazine is the principal pathway of detoxication in soil. Biological dealkylation without dehalogination occurs simultaneously leading to 2-chloro-4-amino-6-isopropylamino-s-triazine (Goswami & Green 1971).
Other information about degradation	Aerobic degradation: OECD screening, 28 d, 9%; closed bottle, 28 d, 13% (Rippen 1988). In surface water, pH 3.8–8.1, 30 d, no degradation (Wolfe 1980). Half-life (total degradation) in 10 years (Dawson et al. 1980). Phytotoxic persistency: 1–3 years (Torstensson 1988). Anaerobic bacteria eliminates original chemical in < 1 day (Jessee et al. 1983). Hydroxyatrazine is the main product of chemical hydrolysis in soil (Goswami & Green 1971).
Bioconcentration factor, fishes	3–10 fish (Verschueren 1983) 2.8 fish (Gunkel & Streit 1980) 3–40 fish (Rudoph & Boje 1988)
Bioconcentration factor, mollusca	3.7 mollusc (Gunkel & Streit 1980)
Bioconcentration factor, algae	10–83 algae (Verschueren 1983)
Bioconcentration factor, other organisms	2–15 snails (Verschueren 1983)
Other information about bioaccumulation	No biomagnification in a model ecosystem (Klaasen & Kadoum 1979).

LD50 values to mammals in oral exposure, mg/kg	1500 orl-rat 750 orl-rbt (Lewis & Sweet 1984) 3080 orl-rat 1750 orl-mus (Martin 1968) 840–880 orl-rat (Rippen 1988)
LD50 values to mammals in non-oral exposure, mg/kg	7500 skn-rbt (Lewis & Sweet 1984) 7500 skn-rbt (Martin 1968)
LC50 values to mammals in inhalation exposure, mg/m³	5200 4 hr, ihl-rat (Lewis & Sweet 1984)
Other information about mammals	In diet: when fed for 2 years to rats at dietary levels of 100 and 1000 ppm, no effect was observed (Martin 1968). NOEL, 28 d, < 30 mg/kg, orl, rat (Rippen 1988). No embryotoxic effect , 1000 mg/kg in birth (Rippen 1988).
Mutagenicity	Negative Ames test and DNA reparation test (Rippen 1988).
Teratogenicity	Teratogenic effect in fish (Birge et al. 1981).
Effects on plants	0.1 mg atrazine/kg soil decreased oat biomass weight by 27.5%. The phytotoxic limiting concentration of atrazine was established as 0.01 mg/kg (Ladonin & Lunev 1983). Lamb's -quarters (Chenopodium album) were killed completely when atrazine was applied with a sprayer at 1.12 kg/ha as preplant incorporation or preemergence or postemergence (Bandeen & McLaren 1976). Avena sativa, EC50, 0.001 mg/kg, TS substrate (Rudoph & Boje 1988).
Effects on microorganisms	Bacteria: Pseudomonas putida: inhibition of cell multiplication starts at > 10 mg/l (Bringmann & Kühn 1976).
EC50 values to algae, mg/l	0.11 96hr, grw, Scenedesmus subspicatus (Geyer et al. 1985) 0.1 rpd, pho, schr, Chlorococcum sp. Isochrysis galbana (Bringmann & Kühn 1976) 0.105 0.04d, oxygen production 0.243 0.04d, oxygen production 0.099 0.04d, oxygen production Cyclotella meneghiniana (Millie & Hersh 1987) 0.1 Chlorella (Rippen 1988) 0.055 Scenedesmus (Böhm 1977)
LOEC values to algae, mg/l	0.003 Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to crustaceans, mg/l	3.6 48hr, Daphnia magna (Kenaga 1979) > 40 act, Daphnia pulex (Nishiuchi & Hashimoto 1967) 1.3 36hr, Procambarus (Rippen 1988)
EC50 values to crustaceans, mg/l	> 39 2d, Daphnia magna (Marchini et al. 1988)
NOEC values to crustaceans, mg/l	0.22 rpd, schr, Daphnia magna (Macek et al. 1976b)

LC50 values to fishes, mg/l	0.87	96 hr, Salmo gairdneri
	0.92	23 days, Salmo gairdneri (embryo)
	0.22–0.34	Ictalurus punctatus (Birge et al. 1979)
	5.4–8.4	2 yr, Lepomis macrochirus
	11–20	1 yr, Pimephales promelas
	4.5–8.8	Salmo gairdneri
	76–100	96 hr, Cyprinus carpio
	16	96 hr, Lepomis macrochirus
	4.0–6.0	1.5yr, Salmo trutta (Macek et al. 1976b)
	15	96hr, Lepomis macrochirus (Klaassen & Kadoum 1979)
	> 10	48hr, Cyprinus carpio (Nishiuchi & Hashimoto 1967)
	26	act, Lepomis macrochirus
	12.6	act, Salmo gairdneri (Kenaga 1979)
LOEC values to fishes, mg/l	0.12	Salmo trutta (Macek et al. 1976b)
	0.16	28d, fish (Rudoph & Boje 1988)
NOEC values to fishes, mg/l	0.065	grw, schr, Salmo trutta
	0.23	Pimephales promelas (Macek et al. 1976b)
	0.054–0.28	Coregonus, grw (Gunkel 1981)
Effects on the physiology of water organisms	Algae; 0.018 mg/l, 12 days; population growth effect (change in cell number of algae species including pre-exponential lag rate effects) (Hamilton et al. 1987). Phaeodactylum tricornutum: 0.015 mg/l, 7 days; growth effect (measurable change in length and/or weight) (Mayasich et al. 1987). Effect on rate of colonization: Algae, 12 d, 0.024–0.134 mg/l (Krieger et al. 1988); aquatic community, 3–21 d, 0.0032 mg/l (Pratt et al. 1988); Protozoa, 3–21 d, 0.0032 mg/l (Pratt et al. 1988). Chlamydomonas reinhardtii: 1–2 d, 0.216 mg/l, lethal effect; 1–2 d, 0.0216 mg/l, change in cell number (Hersh & Crumpton 1987). Lepomis macrochirus, 136 d, 0.020 mg/l, effect on food consumption rate and reproduction (Kettle et al. 1987).	
Other information about water organisms	Algae: Microcystis aeruginosa: inhibition of cell multiplication starts at 0.003 mg/l (Bringmann & Kühn 1976). Algae: Chlorococcum sp. (technical acid): 100 ppb: 50% decrease in 02 evolution 50% decrease in growth; measured as ABS (525 mu) after 10 days Dunaliella tertiolecta (technical acid): 300 ppb: 50% decrease in 02 evolution 50% decrease in growth; measured as ABS (525 mu) after 10 days Isochrysis galbana (technical acid): 100 ppb: 50% decrease in 02 evolution 50% decrease in growth; measured as ABS (525 mu) after 10 days Phaeodactylum tricornutum (technical acid): 100 ppb: 50% decrease in 02 evolution	

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	Phaeodactylum tricornutum (technical acid): 200 ppb: 50% decrease in growth; measured as ABS (525 mu) after 10 days (Walsh 1972). Periphyton ecosystem, inhibited production, 0.08 mg/l (Hamilton et al. 1987). Lemna minor, LC100, 27 d, 0.12 mg/l (Gunkel 1983).
Other information	Not allowed to use in Sweden from 1.1.1990 (Anon. 1989).

183 • Azinphos-ethyl 2642-71-9

Synonyms	0,0-Diethyl-S-(4-oxo-3-H-1,2,3-benzotriazine-3-yl)- methyl-dithiophosphate	
Use	Nonsystemic insecticide and acaricide.	
State and appearance	Colourless crystals.	
Molecular weight	345.4	
Specific gravity (water=1)	1.284	at 20/4 °C
Vapour pressure, mmHg	0.0000002 20 °C	
Melting point, °C	53	
Boiling point, °C	111	at 0.001 mmHg
LD50 values to mammals in oral exposure, mg/kg	7 17.5 12.5	orl-rat (Lewis & Sweet 1984) orl-rat, male orl-rat, female (Martin 1968)
LD50 values to mammals in non-oral exposure, mg/kg	250 250 > 7.5	skn-rat (Lewis & Sweet) skn-rat, 2hr ipr-rat (Martin 1968)
LD50 values to birds in oral exposure, mg/kg	34	orl-ckn (Lewis & Sweet 1984)
LC50 values to crustaceans, mg/l	0.0032 0.004	48 hr, Daphnia pulex 48 hr, Simocephalus serrulatus (Frear et al. 1967)
LC50 values to fishes, mg/l	0.019	96 hr, Salmo gairdneri (Verschueren 1983)

184 • Azinphos-methyl 86-50-0

Synonyms	0,0-Dimethyl-S-((4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl) phosphorodithioate	
Sumformula of the chemical	C10H12N3O3PS2	
Products containing the chemical	Gusation-ruiskutejauhe * azinphos-methyl 250 g/kg	
Use	Active ingredient in insecticides; acaricide; cholinesterase inhibitor.	
State and appearance	Brown waxy solid.	
Odour	Odour threshold: detection: 0.0002 mg/kg water (Sigworth 1964).	
Particle size, mm	0.004 0.1	refuse to the sieve: 6% refuse to the sieve: 0.1% (Gusation *, PESREG)
Molecular weight	317.34	
Specific gravity (water=1)	1.44	at 20/4 °C

Density, kg/m³	1518	at 20 °C (PESREG)
Water solubility, mg/l	29 28	25 °C (PESREG)
Fat solubility, g/100g	4.03	OECD (PESREG)
Melting point, °C	72.4	(PESREG)
Log octanol/water coefficient, log Pow	2.56	(PESREG)

Adsorption/desorption

The adsorption coefficients of azinphos-methyl were determined in aqueous solutions with three soils.

soil type	*% organic carbon*	*Ka*
sandy loam	1.4	3.33
silt loam	1.8	11.04
high organic silt loam	4.6	28.50

(PESREG)

Azinphos-methyl (from 0.13 to 13 ppm) adsorption coefficients determined by the Freundlich equation were 16.75 (silt loam), 7.6 (sandy loam) and 9.85 (silty clay). Desorbed amounts (4 desorption equilbrations) of azinphos-methyl ranged from 32 to 40% (silt loam), 47 to 68% (sandy loam) and 56 to 67% (silt clay). (PESREG)

The adsorption and desorption coefficients and constants of azinphos-methyl were determined in aqueous solutions with four soil types.

	% organic	*adsorption*		*desorption*	
soil type	*matter*	*Ka*	*Koc*	*Kd*	*Koc*
silt loam	2.9	12.7	829	16.9	1102
sandy loam	1.1	4.0	693	6.8	1164
sand	1.0	6.8	1282	9.1	1722
clay loam	2.2	8.4	723	11.7	1006

(PESREG)

Mobility

Rf-values of azinphos-methyl on soil thin-layer plates varies 0.11–0.24 (six different soils). (PESREG)

In soil column study (silt loam soil, aerobic conditions, incubated 28 days, rainfall 45 days, 1.25 cm daily) 4.4% of the applied original radioactivity was found in the leachate. 90% was retained in the upper 5 cm. (PESREG)

The leaching behaviour of azinphos-methyl was studied in the laboratory with and without ageing soil (two different soils). Without prior ageing of the parent compound in the soil about 10–5% of the applied radioactivity were translocated into the leachate of soils. About 0.2–0.3% of unchanged parent compound were recovered from the leachate of both soils. Degradation products were desmethyl azinphos-methyl, hydroxymethyl benzazimide/benzazimide and methyl benzazimide sulfonic acid.

In the study the ageing periods of soils were 30, 62 and 92 days, and rainfall 393 ml/48hr. No parent compound could be detected in the leachate at any time after ageing of the parent compound in the soil. Methyl benzazimidesulfonic acid was the only metabolite being detectable in the leachate (max conc. about 5%). (PESREG)

In the soil column studies azinphos-methyl (1.0–1.25 kg/ha) wasn't found (analysis unit 0.004–0.1 mg/l) in the leachate of six soil samples after two days rainfall (153–200 mm). (PESREG)

	Solubility in organic solvents (g/1000 ml): n-hexane < 1 dichloromethane > 200 2-propanol 1–10 toluene > 200 (PESREG) Decomposition begins at 90 °C and highly exotermic from 110 °C. (PESREG) Dust-air mixture may be explosive, if the is dust over 500 g/m³ in the air. (Gusation *, PESREG)
Photochemical degradation in soil	The photolysis (high intensity mercury lamp) half-life of (C-14) azinphos-methyl in a sandy loam soil was 9 days. The photolysis products were benzazimide and/or hyrdoxymethyl benzazimide (after 10 days 4%), azinphos-methyl oxygen analog, methyl benzazimide and bis-(benzazimide-N-methyl) sulfide. (PESREG) Azinphos-methyl (3.38 kg/ha) was irradiated with natural sunlight. 80% of the parent was recovered after 31 days exposure. The estimated half-life of azinphos-methyl under these study conditions was 99 days. (PESREG)
Photochemical degradation in water	The photo lysis (high intensity mercury lamp) half-life of (C-14) azinphos-methyl in an aqueous solution (pH 4) was 9.4 hours. The photolysis products were benzazimide and/or hyrdoxymethyl benzazimide (after 48 hours about 40%), anthranilic acid (after 48 hours about 10%) and methyl benzazimide. No volatile degradation products were formed. (PESREG) Aqueous azinphos-methyl (10.3 ppm) was irradiated with natural sunlight. The half-life was 76.7 hours. Photo lysis products were benzazimide and anthranilic acid. (PESREG)
Hydrolysis in water	The half-lives of azinophos-methyl in water and on glass beads:

	half-lives (days)				
		in water		*dry glass*	*wet glass*
temp	*pH 8.6*	*pH 9.6*	*pH 10.7*	*beads*	*beads*
6 °C	36.4	4.95	3.9	99	91
25 °C	27.9	2.40	2.0	66	10
40 °C	7.2	0.65	0.41	48	1

(PESREG)

The half-life of azinophos-methyl was 23.1 days (30 °C) and 50 days (calc.) (22 °C) at pH 7. (PESREG)

The hydrolysis half-lives of azinophos-methyl in buffer solutions:

pH	*concentration (ppm)*	*temperature (°C)*	*half-life (days)*
4	1	30	39
4	10	30	42
4	1	40	18
4	10	40	21
7	1	30	23
7	10	30	25
7	1	40	11
7	10	40	12
9	1	30	2.2
9	10	30	2.5
9	1	40	1.1
9	10	40	1.3

The major hydrolysis products were
pH 4, 7 and 9 benzazimide and/or hydroxymethyl benzazimide; bis-(benzazimide-N-methyl) sulfide;
pH 4 and 7 mercaptomethyl benzazimide;
pH 7 and 9 anthranilic acid.
(PESREG)

Hydrolysis in acid	The half-life of azinophos-methyl was 38.9 days (30 °C) and 87 days (calc.) (22 °C) at pH 4. (PESREG)
Hydrolysis in base	The half-life of azinophos-methyl was 2.2 days (30 °C) and 4.1 days (calc.) (22 °C) at pH 9. (PESREG)
Half-life in water, days	12.8 pH 8.8, 20 °C (de Heer 1979) 55 pH 7.6, 20 °C (de Heer 1979)
Aerobic degradation in soil	The degradation behaviour of azinphos-methyl was studied in the laboratory under aerobic conditions with two soils. After an incubation period of 30 days about 6.8–8.6% of applied active ingredient could be extracted from the soils. After 92 days the proportion of parent compound was about 4.6–6.2%. The following degradation products were detected: desmethyl azinphos-methyl; hydroxymethyl benzazimide/benzazimide; methylsulfinyl-methyl-benzazimide; methylsulfonyl-methyl benzazimide; methyl benzazimide sulfonic acid. (PESREG) The degradation of azinphos-methyl was investigated in sandy loam soil under aerobic conditions. The degradation rate of azinphos-methyl did not follow strictly first order kinetics over the 365 day period. A half-life value can be estimated for azinphos-methyl through 95% degradation and was shown to be 44 days. The degradation products were azinphos-methyl oxygen analog, mercaptomethyl benzazimide, benzazimide and/or hydroxymethyl benzazimide and bismethyl benzazimide sulfide. (PESREG) The half-life of azinphos-methyl in sterile soil (sandy loam soil) was 355 days. (PESREG) The degradation of azinphos-methyl was studied in the laboratory tests on two different soils. Approx. 19–9% of the C-14 activity applied was eliminated as 14CO2 222–552 days after application of (carbonyl-C-14) azinphos-methyl. Also the degradation of (phenyl-UL-C-14) azinphos-methyl was studied in the soil. Approx. 10% of the applied C-14 activity was eliminated as 14CO2 365 days after application. (PESREG)
Anaerobic degradation in soil	The half-life of azinphos-methyl under anaerobic soil (sandy loam soil) conditions was 68 days following 30 days in aerobic soil. No additional metabolites were formed under anaerobic conditions. (PESREG)
Degradation and transformation products	Azinphos-methyl oxygen analog; Benzazimide and/or hydroxymethyl benzazimide; bis-(benzazimide-N-methyl) sulfide; mercaptomethyl benzazimide; anthranilic acid.
Other information about degradation	The major metabolic pathway in the degradation of azinphos-methyl is hydrolysis of the phosphorous ester resulting in mercaptomethyl benzazimide or hydroxymethyl benzazimide and their dimethyl (mono or di) thiophosphoric acids. Minor metabolic pathways are 1) oxidative desulfurization with formation of azinphos-methyl oxygen analog, 2) hydrolysis of the phosphorous-methoxy group to yield either desmethyl azinphos-methyl or desmethyl oxygen analog and 3) isomerization of the methoxy-oxygen and phosphorothiono-sulfur to ultimately give the desmethyl azinphos-methyl S-methyl isomer; further degradation of these products occurs by hydrolysis of the phosphorous ester linkage between the phosphorus and the benzazimide moiety. Azinphos-methyl oxygen analog is the only metabolite/degradation product which exhibits cholinesterase inhibition activity. Azinphos-methyl itself shows only slight activity. (PESREG)
Bioconcentration factor, fishes	60 appr. 60, exposure 15 ppb, 28d Ictalurus punctatus (PESREG)

A

LD50 values to mammals in oral exposure, mg/kg	11 orl-rat (Lewis & Sweet 1984) 80 orl-gpg, male (Martin 1968) 13–16.4 orl-rat (Anon. 1976) 4.4–4.6 orl-rat > 10 orl-dog 6.7 orl-rat male not fed 12.8 orl-rat male fed 15.5 orl-rat male 9.1 orl-rat male not fed 17.25 orl-rat male fed 25.4 orl-rat male 12.2–15 orl-rat female 10–19 orl-rat 5.6 orl-rat male 6.4 orl-rat female (PESREG) 58 orl-rat male, Gusation * 53 orl-rat female, Gusation * (PESREG)
LD50 values to mammals in non-oral exposure, mg/kg	65 skn-mus 220 skn-rat (Lewis & Sweet) 220 skn-rat (Anon. 1976) 200–250 idr-rat male 155 idr-rat female (PESREG) 8.5–8.9 ipr-rat female (PESREG)
LC50 values to mammals in inhalation exposure, mg/m³	155 4hr, ihl-rat male 132 4hr, ihl-rat female 396 1hr, ihl-rat male 310 1hr, ihl-rat female (PESREG)
Other information about mammals	In diet; no mortality occurred in rats fed 1 mg/kg/day for 60 days (Martin 1968).
Carcinogenicity	NCI carcinogenesis bioassay completed: results indefinite, rat; results negative, mus (Lewis & Sweet 1984).
LD50 values to birds in oral exposure, mg/kg	136 orl-dck 277 orl-ckn (Lewis & Sweet 1984) 8.00–8.50 orl-Agelaius phoeniceus 27 orl-Sturnus vulgaris (Schafer et al. 1983) 32 14d, orl-Colinus virginianus, GLP (PESREG)
NOEC values to birds in oral exposure, mg/kg	5.6 NOEL, 14d, Colinus virginuanus, GLP (PESREG) 12 20w-diet, Anas platyrhyncos, GLP (PESREG)
Effects on the reproduction of birds	The no-reproduction-effect concentration is 35 ppm, 20 week-diet Anas platyrhyncos. There was apparent treatment-related decrease in the percent hatched, 101 ppm, 20 week-diet, Anas platyrhyncos.GLP (PESREG)
Other information about birds	LOEC is 35 ppm based on the decresed body weight gains of the adult Anas platyrhyncos in 20 week-diet. GLP (PESREG)

Effects on invertebrates	LC50, 59 mg/kg, 14d, Eisenia foetida, OECD No 207 LLC, 32 mg/kg, 14d Eisenia foetida, OECD No 207 NOEC, 1 mg/kg, 14d, Eisenia foetida, OECD No 207 (PESREG)
Effects on bees	LD50, 0.000063 mg/bee, 460 g a.i./ha (Smart & Stevenson 1982) LD50, 0.000423 mg/bee, 48hr, at 26.7 °C (Atkins & Anderson 1967)
Effects on arthropods	Pteronarcys dorsata: 0.0211 mg/l, 96hr LC50; 0.0049 mg/l, 30d LC50 Acroneuria lycorias: 0.0015 mg/l, 30d LC50; 0.00136 mg/l, 30 day, no effect Ophiogomphus rupinsulensis: 0.012 mg/l, 96hr LC50; 0.0022 mg/l, 30d LC50; 0.00173 mg/l, 30d, no effect Hydropsyche bettoni: 0.0074 mg/l, 30d LC50; 0.00494 mg/l, 30d no effect Ephemerella subvaria: 0.0045 mg/l, 30d LC50; 0.0025 mg/l, 30d, no effect (Verschueren 1983). Pteronarcys californica: 0.0015 mg/l, 96hr LC50 (Sanders & Cope 1968).
Effects on microorganisms	Significant differences were recognized on soil respiration between azinphos-methyl treated and untreated soil:

soil	*mg azinphos-methyl /kg in soil*	*days after treat-ment*	*soil respiration significant difference carbon dioxide*
LOAMY SAND			
without lucerne-grass	1.07	7	+
	10.67	7	+
	1.07	14	+
	10.67	21	+
with lucerne-grass	1.07	7	+
	1.07	14	+
	10.67	14	+
	1.07	21	+
	10.67	21	+
SANDY SILT			
without lucerne-grass	10.67	7	+
	1.07	14	+
	10.67	14	+
with lucerne-grass	1.07	21	+

(PESREG)

Significant differences in mineralization of nitrogen were observed between azinphos-methyl treated and control soil samples:

soil	*mg azinphos-methyl /kg in soil*	*days after treat-ment*	*significant difference ammonium*	*nitrate*
loamy sand	1.07	0	+	+
	1.07	7		+
	10.67	7		+
	1.07	14		+
	10.67	14		+
	1.07	21	+	+
	10.67	21	+	+
	1.07	28		+
	10.67	28		+
	1.07	42		+
	10.67	42		+
	1.07	56		+
	10.67	56		+
sandy silt	1.07	14		+
	10.67	14		+
	10.67	42		+
loamy sand after amendment with ammonium	1.07	21	+	+
	10.67	21	+	+
	1.07	28	+	
	10.67	28	+	
sandy silt after amendment with ammomium	1.07	0		+
	10.67	0		+
	1.07	14	+	+
	10.67	56	+	+

(PESREG)

Azinphos-methyl (at 2 to 10000 ppm) did not inhibit the bacteria and actinomycetes, but it (at 2 to 10 ppm) caused 4 to 18% inhibition of the four fungi (Aspergillus niger, Penicillium daleae, Trichoderma viride and Phycomyces nitens). (PESREG)

EC50 values to algae, mg/l	3.61	96hr, EbC50, grw ihb
	7.15	96hr, ErC50, grw ihb Scenedesmus subspicatus OECD No 201 (PESREG)
LC50 values to crustaceans, mg/l	0.00019	Daphnia magna)
	0.00019	act, Daphnia pulex (Frear et al. 1967
	0.00015	96 hr, Gammarus lacustris
	0.0001	96 hr, Gammarus fasciatus (Sanders 1969)
	0.00016	20 d, Palaemonetes kadiakensis
	0.021	96 hr, Asellus brevicaudus
	0.0032	act, Daphnia pulex
	0.0012	120 hr, Palaemonete kadiakensis (Kenaga 1979)
	0.0011	48hr, Daphnia magna (PESREG)
	0.0003	48hr, Mysidopsis bahia, GLP (PESREG)
	0.00022	96hr, Mysidopsis bahia, GLP (PESREG)
	0.0001	96hr, Gammarus fasciatus
	0.021	96hr, Asellus Brevicaudus (de Heer 1979)

EC50 values to crustaceans, mg/l	0.003	srv, 48 hr, Daphnia pulex (Shapiro 1979)
NOEC values to crustaceans, mg/l	< 0.00013	96hr, Mysidopsis bahia GLP (PESREG)
LC50 values to fishes, mg/l	3.29	96hr, Ictalurus punctatus
	0.013	96hr, Perca flavescens
	0.017	96hr, Oncorhynchus kisutch
	0.004	96hr, Salmo trutta
	0.005	96hr, Micropterus salmoides
	0.052	96hr, Lepomis microlophus
	0.014	96hr, Salmo gairdneri (Macek & McAllister 1970)
	0.17	96 hr, Rasbora heteromorpha (Tooby et al. 1975)
	0.093	96hr, Pimephales promelas
	4.3	96hr, Carassius auratus
	0.24	96hr, Phoxinus phoxinus
	0.7	96hr, Cyprinus carpio
	0.02	96hr, Lepomis macrochirus (Katz 1961)
	0.24	96hr, Pimephales promelas
	> 1	96hr, Carassius auratus
	0.1	96hr, Poecilia reticulata
	0.052	Lepomis macrohirus (Kenaga 1979)
	0.3	96 hr, Pimephales promelas
	0.022	96 hr, Lepomis macrochirus
	0.013	96 hr, Perca flavescens (Kemp et al. 1973)
	7.1	96hr, Salmo gairdneri, fingerlings (Marking & Mauck 1975)
	1.04	4d, Carassium auratus
	3.22	4d, Ictalurus punctatus
	0.0093	4d, Lepomis macrochirus
	0.065	4d, Pimephales promelas
	0.0091	4d, Salmo gairdneri (Holcombe et al. 1987)
	0.003	96hr, Salmo gairdneri, GLP
	0.12	96hr, Leuciscus idus melanotus
	0.0027	96hr, Cyprinodon variegatus, GLP
	0.00233	21d, Salmo gairdneri, OECD No 204
	0.00091	47d, srv, lrv, Salmo gairdneri, GLP (PESREG)
	0.1	96hr, Lebistes reticulatus (de Heer 1979)
EC50 values to fishes, mg/l	0.00067	47d, bms rcd, Salmo gairdneri, GLP (PESREG)
LOEC values to fishes, mg/l	0.0005	rpd, chr, Pimephales promelas (Adelman 1976)
	0.00085	21d, Salmo gairdneri, OECD No 204 (PESREG)
NOEC values to fishes, mg/l	0.0003	rpd, chr, Pimephales promelas (Adelman 1976)
	0.00091	96hr, Cyprinodon variegatus, GLP
	0.001	96hr, Salmo gairdneri, GLP
	0.00039	21d, Salmo gairdneri, OECD No 204 (PESREG)
	0.00023	srv, lrv, 60d post-hatch, Salmo gairdneri, GLP (PESREG)

Other information about water organisms	Crustacean: Gammarus pseudolimneaus: 0.00010 mg/l, 30 day, no effect (Sanders 1972). Aplexa hypnorum: LC50, 4 d, > 3.69 mg/l (Holcombe et al. 1987). Mollusca: EC50, 96hr, 4.7 mg/l, Crassostrea virginica NOEC, 96hr, 2.0 mg/l, Crassostrea virginica EPA (PESREG) Salmo gairdneri, larvae: 0.00098 mg/l, 60 days post-hatch, 25% larvae survival. The maximum acceptable toxicant concentration of azinphos-methyl for Salmo gairdneri was estimated to be > 0.00044 mg/l and < 0.00098 mg/l. GLP (PES-REG) Salmo gairdneri (early life stages), 47 days: The maximum acceptable toxicant concentration was 0.00029 mg/l. (PESREG) Based on the statistical analysis of adult mean length, survival and young/adult/reproduction day from the 21-day Daphnia magna dynamic life cycle study, the MATC (maximum acceptable toxicant concentration) limits were estimated to be (C-14) azinphos-methyl mean measured concentrations of 0.00025 and 0.00040 mg/l (PESREG).

185 • Azobenzene 103-33-3

Synonyms	Diphenyldiimide Benzeneazobenzene
Sumformula of the chemical	C12H10N2
Use	Manufacture of dyes and rubber accelerators; fumigant; acaricide.
State and appearance	Yellow or orange crystals.
Molecular weight	182.23
Specific gravity (water=1)	1.09
Melting point, °C	68.3
Boiling point, °C	293
Log octanol/water coefficient, log Pow	3.82 (Sangster 1989)
Other information about degradation	Impact on biodegradation processes: at 100 mg/l no inhibition of NH3 oxidation by Nitrosomonas sp. (Hockenbury & Grady 1977).
Other information about mammals	In diet: dogs fed 63 days on diet containing 600 ppm, suffered high mortality and liver damage (Martin 1968).
Mutagenicity	Mutagenicity in the Salmonella test: positive 1.4 revertant colonies/nmol 379 revertant colonies at 0.050 mg/plant (McCann et al. 1975).
LD50 values to birds in oral exposure, mg/kg	> 98.0 orl-Agelaius phoeniceus (Schafer et al. 1983)

186 • Azoic CC2 92-77-3

Sumformula of the chemical	C17H13NO2
EINECS-number	2021881
Water solubility, mg/l	< 50 (MITI 1992)
Melting point, °C	243–244 (MITI 1992)

Total degradation in water	Biodegradation: 5.4% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.59–5.9 < 6.5	6w, Cyprinus carpio, conc 0.5 mg/l 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 100	48hr, Oryzias latipes (MITI 1992)

187 • Azoic CC5

91-96-3

Sumformula of the chemical	C22H24N2O4	
EINECS-number	2021111	
Water solubility, mg/l	3.5	(MITI 1992)
Melting point, °C	208	(MITI 1992)
Log octanol/water coefficient, log Pow	1.75	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.2 < 1.6	6w, Cyprinus carpio, conc 1 mg/l 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 500	48hr, Oryzias latipes (MITI 1992)

188 • Bandane

8029-29-6

Use	Herbicide.
Effects on plants	Severe thinning of bermudagrass occurred with bandane at 34 kg ai/ha, which also gave complete control of crabgrass following nine consecutive annual applications (Callahan 1980).

189 • Barban

101-27-1

Use	Herbicide.	
EC50 values to micro–organisms, mg/l	24.2 27.5 26.2 35 27.8	DIDHA, ethanol (Bitton et al. 1986) DIDHA, DMSO (Bitton et al. 1986) DIDHA (Bitton et al. 1986) INT (Bitton et al. 1986) DIDHA (Bitton et al. 1986)
LC50 values to fishes, mg/l	0.91	48hr, Rasbora heteromorpha (Kemp et al. 1973)

190 • Barium and barium compounds 7440-39-3

LC50 values to fishes	410 13.5 14.5	48hr, Daphnia magna (LeBlanc 1980) 21d, Daphnia magna 48hr, without food, D.magna (Biesinger & Christensen 1972)
EC50 values to crustaceans, mg/l	8.9	rpd, schr, 21 d, Daphnia magna (Biesinger & Christensen 1972)
LOEC values to crustaceans, mg/l	5.8	rpd, schr, 21 d, Daphnia magna (Biesinger & Christensen 1972)
LC50 values to fishes, mg/l	42.7	28d, Salmo gairdneri (Birge et al. 1980)

191 • Barium sulfate 7727-43-7

LC50 values to fishes, mg/l	76000	96 hr, Salmo gairdneri (Sprague & Logan 1979)

192 • Basic Yellow-2 2465-27-2

Synonyms	Benzenamine, 4,4'-carbonimidoylbis[N,N-dimethyl-, monohydrochloride Auramine hydrochloride	
Sumformula of the chemical	C17H21N3.ClH	
EINECS-number	2195672	
Water solubility, mg/l	10000	(MITI 1992)
Melting point, °C	271–274 (MITI 1992)	
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l, (MITI 1992).	
Bioconcentration factor, fishes	3.8–11 6.1–16	6w, Cyprinus carpio, conc 0.1 mg/l 6w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	5.3	48hr, Oryzias latipes (MITI 1992)

193 • Bayer 16574 3568-51-2

Other information about mammals	LDfr = 25.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

194 • Bayer 20172 5902-46-5

Other information about mammals	LDfr = 75.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

B

195 • Bayer 22684

3212-19-9

Other information about mammals	LDfr = 25.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

196 • Bayer 25918

115-91-3

Other information about mammals	LDfr = 50.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

197 • Bayer 28580

728-40-5

Other information about mammals	LDfr = 85.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

198 • Bayer 29491

2951-17-9

Other information about mammals	LDfr = 12.5 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

199 • Bayer 29952

2703-13-1

Other information about mammals	LDfr = 50.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

200 • Bayer 30237

3186-14-9

Other information about mammals	LDfr = 75.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

201 • Bayer 30468

3186-12-7

Other information about mammals	LDfr = 62.5 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

202 • Bayer 30749

2636-23-9

Other information about mammals	LDfr = 28.1 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

203 • Bayer 30750

3309-71-5

Other information about mammals	LDfr = 25.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

204 • Bayer 30911

2667-49-4

Other information about mammals	LDfr = 25.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

205 • Bayer 34042 3568-56-7

Synonyms	Bay 34042
Other information about mammals	LDfr = 6.25 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).
LD50 values to birds in oral exposure, mg/kg	< 0.316 orl-Agelaius phoeniceus 1.78 orl-Sturnus vulgaris (Schafer et al. 1983)

206 • Bayer 37343 3506-28-3

Other information about mammals	LDfr = 87.5 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

207 • Bayer 46676 25537-46-6

Other information about mammals	LDfr = 25.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

208 • Bayer 47043 922-86-1

Other information about mammals	LDfr = 62.5 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

209 • Bayer 47416 2830-86-6

Other information about mammals	LDfr = 62.5 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

210 • Bayer 47940 63981-11-3

Other information about mammals	LDfr = 37.5 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

211 • Bayer 51896 25918-54-1

Other information about mammals	ALD = 42.0 mg/kg, act, orl, deer mouse; LDfr = 62.5 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

212 • Bayer 51937 82980-43-6

Other information about mammals	ALD = 62.0 mg/kg, act, orl, deer mouse; LDfr = 25.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

213 • Bayer 52752 82980-44-7

Other information about mammals	ALD = 62.0 mg/kg, act, orl, deer mouse; LDfr = 87.5 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

B

214 • Bayer 52957

4156-44-9

Other information about mammals	LDfr = 62.5 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

215 •Bayer 56200

82679-90-1

Other information about mammals	ALD = 62.0 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987).

216 • Bayer 56301

1156-52-1

Other information about mammals	ALD = 28.0 mg/kg, act, orl, deer mouse; LDfr = 25.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

217 • Bayer 56582

7205-22-3

Other information about mammals	ALD = 62.0 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987).

218 • Bayer 60564

64205-22-7

Other information about mammals	ALD = 94 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987).

219 • Bayer 60737

1970-15-6

Other information about mammals	ALD = 94.0 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987). LDfr = 62.5 mg/kg/day, subacute, deer mouse.

220 • Bayer 60738

2799-95-3

Other information about mammals	ALD = 62.0 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987).

221 • Bayer 60830

82980-46-9

Other information about mammals	ALD = 8.0 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987).

222 • Bayer 61035

1804-58-6

Other information about mammals	ALD = 94 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987).

B

223 • Bayer 73 — 50-65-7

Synonyms	5-Chloro-2'-chloro-4'-nitrosalicylanilide
Use	Lampricide.
LC50 values to fishes, mg/l	0.049 24hr, Petromyzon marinus (Rye & King 1976) 0.5 Gambusia affinis (Karim et al. 1987)
Effects on the physiology of water organisms	Grocothemis eryhraea, 30 mg/l, stress (Karim et al. 1987).
Other information about water organisms	Lanistes carinatus, LC50, 0.295 mg/l (Karim et al. 1987).

224 • Bayer 91273 — 25205-08-7

Other information about mammals	ALD = 18 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987).

225 • Bayluscide — 1420-04-8

Synonyms	Niclosamide
LD50 values to birds in oral exposure, mg/kg	> 96 orl-Agelaius phoeniceus (Schafer et al. 1983)
LC50 values to fishes, mg/l	0.62 4 d, Clarias lazera (Faisal et al. 1988)
Other information about water organisms	Lethal effect: 0.33 d, 0.8 mg/l, Biophalaria alexandrina 0.33 d, 0.8 mg/l, Bulinus truncatus 0.13 d, 0.5 mg/l, Lymnaea natalensis 0.13 d, 3.0 mg/l, Physa acuta (Abdel-Rahman et al. 1988). Mortality. 0.58 d, < 0.010–0.573 mg/l: Micropterus salmoides; Salmo gairdneri (Ho & Gloss 1987).

226 • Behenic acid — 112-85-6

Synonyms	Docosanoic acid n-Docosoic acid
Sumformula of the chemical	CH3(CH2)20COOH
Use	Cosmetics; waxes, plasticizers; stabilizers.
Molecular weight	340.58
Specific gravity (water=1)	0.8221 at 100/4 °C
Water solubility, mg/l	1000 at 10 °C
Melting point, °C	80.2
Boiling point, °C	306 at 60 mm
Other information	Natural sources: a minor component of the oils of the type of peanut and rape-see.

227 • Bendiocarb

22781-23-3

LC50 values to crustaceans, mg/l	5.55	4d, Procambarus clarkii (Holck & Meek 1987)
Other information about water organisms	Anopheles quadrimaculatus, 1 d, 0.081 mg/l, LC50 (Holck & Meek 1987).	

228 • Benomyl

17804-35-2

Synonyms	Methyl-1-(butylcarbamoyl)-2-benzimidazole-carbamate	
Use	Active ingredient in fungicides. In agriculture as a systemic fungicide for controlling a broad spectrum of phytopathogenic fungi including rice pathogens.	
Molecular weight	290.36	
Total degradation in water	Benomyl is transformed readily to methyl-2-benzimidazole carbamate (MBC) and 2-aminobenzimidazole (AB) in soils and in water (Verschueren 1983).	
LD50 values to mammals in oral exposure, mg/kg	10000	orl-rat
	5600	orl-mus (Lewis & Sweet 1984)
	> 10000	orl-rat (Anon. 1976)
LD50 values to birds in oral exposure, mg/kg	100	orl-bwd (Lewis & Sweet 1984)
	100	orl-Agelaius phoeniceus
	> 100	orl-Sturnus vulgaris (Schafer et al. 1983)
Effects on plants	Growth of mycorrhizal sour orange (Citrus aurantium) seedlings was depressed by spraying of soil with 11.2 kg benomyl (50%)/ha. * (Nemec 1980)	
EC50 values to algae, mg/l	1.4	rpd, act,48 hr, Chlorella pyrenoidosa (Canton 1976)
LC50 values to crustaceans, mg/l	0.64	48 hr, Daphnia magna (Canton 1976)
LC50 values to fishes, mg/l	0.17	96 hr, Salmo gairdneri (Pesticide Manual 1983)
	1.8	72 hr, Salmo gairdneri
	190	72 hr, Cyprinus carpio
	110	72 hr, Poecilia reticulata (Hejduk & Svobodova 1980)
	48	48 hr, Salmo gairdneri (Canton 1976)
	4.2	96 hr, Carassius auratus (Pesticide Manual 1983)

229 • Bensulide

741-58-2

Use	Selective preemergence herbicide.	
State and appearance	Amber-coloured liquid.	
Specific gravity (water=1)	1.23	at 20/20 °C
LD50 values to mammals in oral exposure, mg/kg	1082	orl-rat, male (Anon. 1976)
	339	orl-rat, male, albino (Martin 1968)
LD50 values to mammals in non-oral exposure, mg/kg	3950	skn-rat, albino (Martin 1968)
Other information about mammals	In diet: well tolereted by rats and dogs fed 90 days at dietary levels up to 250 ppm and 625 ppm, respectively (Martin 1968).	

Effects on plants	Bensulide at 11 kg ai/ha gave complete control of crabgrass following nine consecutive annual applications (Callahan 1980).	
LC50 values to crustaceans, mg/l	1.4	96 hr, Gammarus fasciatus (Kemp et al. 1973)
LC50 values to fishes, mg/l	0.38	96 hr, Ictalurus punctatus (McCorkle et al. 1977)

B

230 • Bentazone 25057-89-0

Synonyms	3-Isopropyl-1H-2,1,3-benzothiadiazin-(4)3H-one-dioxide
Use	Active ingredient in herbicides.
Effects on plants	1.0 kg bentazon/ha was applied with a sprayer 24 days after seeding to lamb's-quarters (Chenopodium album L.) in the 3 to 4-leaf stage — atrazine-susceptible plants (seeds) were killed and there was a decrease in shoot growth and plant number of atrazine-resistant plants (Jensen et al. 1977).

231 • Benz(a)acridine 225-11-6

Molecular weight	229	
Log octanol/water coefficient, log Pow	4.45	calc.
Bioconcentration factor, crustaceans	352	initial conc. 18 ppb, Daphnia pulex (Verschueren 1983)
LC50 values to crustaceans, mg/l	0.449	24hr, Daphnia pulex (Verschueren 1983)

232 • Benz(a)anthracene 56-55-3

Synonyms	B(a)A 1,2-Benzanthracene Benzo(a)anthracene 2,3-Benzphenanthrene Tetraphene Benzanthrene Naphthantracene Benzo(b)phenanthrene	
Sumformula of the chemical	C18H12	
Use	Occurs in coal tar, gasoline, and diesel engine exhaust, cigarette smoke, flue gases from coal-fired installations and municipal incinerators, and foods.	
State and appearance	Colourless leaflets with yellow-green fluorescence.	
Molecular weight	228.3	
Vapour pressure, mmHg	0.0000000050 mmHg, 25 °C	
Water solubility, mg/l	0.01 0.044	 practical grade, at 24 °C
Boiling point, °C	400	760 mmHg
Sublimation point, °C	160	
Log octanol/water coefficient, log Pow	5.61 5.61 5.91	(Sax 1986) (Mackay 1982) (Sangster 1989)

Volatilization	Volatilization has a half-life of about 90 hr and is probably not as important a transport process as adsorption. Evaporation of lower-molecular-weight PAHs may be significant only in a clear, rapidly flowing shallow stream (Sax 1986).
Adsorption/desorption	Aquatic reactions: adsorption: in estuarine water: at 0.010 mg/l, 53% adsorbed on particles after 3 hours (Lee 1977). Movement in sediment is an important transport process. The partition coefficient for benz(a)anthracene between water and sediment containing 50% organic carbon was estimated to be 21000. The one-compartment model predicted that 71% will be sorbed onto suspended sediments. – In experiments, with radio-labelled PAHs, the percentage of sorbed benz(a)anthracene in various surface waters and waste waters was 19–60% at 22 °C. The log of the mean partition coefficient between the suspended particulates and the water was 4.52. The half-life of benz(a)anthracene in a typical river due to bottom sediment sorption only is estimated to be 40 hours. – An exchange equilibrium exists in natural water systems between absorbed and soluble PAHs. Although the particulate form is favoured, a significant fraction of the PAH will be dissolved except in systems that are very heavily contaminated by PAHs (Sax 1986).
Other bindings	After 3 hours incubation in natural seawater, 59% of 0.003 mg/l were taken up by suspended aggregates of dead phytoplankton cells and bacteria (Lee et al. 1978). Insoluble in water.
Photochemical degradation in air	Reaction with ozone gives benzanthracene-7,12-dione. Oxidation with lead tetracetate gives the 7-acetoxy derivative. It reacts with dienes. It adds maleic anhydride across the 7,12-position. – Besides oxidation products such as the quinones, diacids, and nucleas and side-chain oxidation products, chlorinating agents also produce chlorine-substituted polycyclic aromatic hydrocarbons. – The most common photo oxidation product of PAHs in solution in an endo peroxide. Dealkylation, ring cleavage, and other reactions ensue following photo lysis or pyrolysis of these peroxides. Frequently, only quinones are isolable. Photo dimers may result in some cases. Adsorbed PAHs are more reactive than in solution (Sax 1986).
Photochemical degradation in water	The dissolved portion may undergo photo lysis with a half-life of 10 to 50 hours. The portions suspended or absorbed on mineral surfaces may also undergo rapid photo oxidation. The half-life tor photo lysis was 0.59 hours, calculated for surfce waters in midsummer at 40° N latitude (Sax 1986).
Hydrolysis in water	Benz(a)anthracene does not hydrolyse (Sax 1986).
Oxidation-reduction reactions	Oxidation by RO2 radicals is slow with a half-life of 38 hr and is not a significant fate process. Chlorine and ozone used in drinking water disinfection oxidize PAHs to quinones. The half-life for benz(a)anthracene with ozone in water is approximately 27 minutes. The half-life for the reaction of chlorine with all PAHs is less than 0.5 hr (Sax 1986).
Half-life in air, days	15.3 with ozone in the gas phase (Sax 1986)
Half-life in water, days	0.023 0.55hr, in a stream 0.917 22hr, in an eutrophic pond or lake (Sax 1986)
Aerobic degradation in water	Biodegradation to CO2 in estuarine water:

conc. mg/l	*month*	*incubation time (hr)*	*degradation rate (mg/l/day) x 1000*	*turnover time (days)*
0.010	January	48	0	-
0.010	June	48	0	-

(Lee 1977).

Total degradation in sediment	PAHs deposited in sediments are less subject to photochemical or biological oxidation, especially if the sediment is anoxic. Sedimentary PAH is therefore quite persistent and may accumulate to high concentrations (Sax 1986).

Other information about degradation	Biodegradation was not observed during enrichment procedures (Verschueren 1983). Airborne particulate PAHs can persist at relatively high concentrations in aerosols transported for long distances. The atmospheric persistence is longer than would be predicted from laboratory photo oxidation studies. On the other hand, The National Academy of Sciences (1972) proposed that the chemical half-life of PAH's in the atmosphere may be limited to hours or days (Sax 1986). Biodegradation is probably the ultimate fate process for benz(a)anthracene (Sax 1986). The half-lives for microbial transformation of benz(a)anthrecene were 1400 and 100 for water and sediment, respectively, with a high PAH level; 7000 hr for a sediment with a moderate PAH level and > 20000 for sediment with a low PAH level. – Most species cannot use PAHs as a sole carbon source. Microbial oxidation of PAHs requires oxygen and will not proceed in anoxic sediments or water (Sax 1986).
Other information about metabolism	There are large differences among aquatic species in their ability to absorb and assimilate PAH from food. Polychaete worms have a very limited ability; fish show limited and variable absorption from the gut; and crustaceans readily assimilate PAH. Assimilated PAHs are metabolized and excreted rapidly. For biomagnification to occur, a substance must be relatively resistant to metabolism or exretion (Sax 1986).
Bioconcentration factor, mollusca	530 — 2 days, Crassostrea virginica 18000 — 8 days, Crassostrea virginica (Lee et al. 1978)
Bioconcentration factor, crustaceans	10000 — Daphnia pulex (Sax 1986)
Bioconcentration factor, other organisms	11700 — steady-state, aquatic organisms containing 7.6% lipids (Sax 1986)
Other information about bioaccumulation	Bioaccumulation is a short-term process. Polyaromatic hydrocarbons with 4 or fewer aromatic rings are readily metabolized by multicellular organisms and degrades by microbes. In most cases, PAHs are less bioavailable when complexed to colloidal organic materials or adsorbed to organic or inorganic particulated than when in solution or in fine dispersion in water (Sax 1986).
LDLo values to mammals in non-oral exposure, mg/kg	10 — ivn-mus (Lewis & Sweet 1984)
TDLo values to mammals in non-oral exposure, mg/kg	18 — skn-mus, tumorigenic 2 — scu-mus, tumorigenic 80 — imp-mus, tumorigenic (Sax 1986)
Health effects	Direct contact: Skin contact with benz(a)anthracene in solvents causes local tumors in some species. Acute hazard level: Carcinogenic. PAHs can presumably be absorbed from ingestion, inhalation, and skin contact.
Carcinogenicity	Carcinogenic (McCann et al. 1975). Benz(a)anthracene has proved carcinogenic in the mouse by several routes of administration, but it has not been adequately tested in other species. It produced hepatomas and lung adenomas in young mice following repeated oral dosing. It is a complete carcinogen for the mouse skin and is also an initiator of skin carcinogenesis in mice. Subcutaneous injections of doses as low as 0.050 mg procuces tumors in adult and newborn mice. Its implantation in mice produced bladder tumors. No case reports of epidemiological studies relating to the carcinogenic risk of benz(a)anthracene in humans are available, but it is present in coal tar and other materials known to be human carcinogens (Sax 1986).

Mutagenicity	Mutagenicity in the Salmonella test: positive; 11 revertant colonies/nmol 2640 revertant colonies at 0.057 mg/plate (McCann et al. 1975). Benz(a)anthracene metabolites are mutagenic to human cells in culture, drosophila, rodent cells in culture, and bacteria. – Benz(a)anthracene in the micronucleus test and the chromosome aberrations test induced mutations in spermatogonia and bone marrow cells of hamsters ans in NMRI mice oocytes (Sax 1986).
Effects on wastewater treatment	Polychlorinated PAHs are probably highly toxic to aquatic organisms and persistent in the environment as are polychlorinated biphenyls and polychlorinated naphthalenes. Chlorination for purification of wastewaters or drinking waters containing high concentrations of PAHs may be inadvisable. Activated sludge treatment is unable to oxidize PAHs within normal retention times (Sax 1986).
LC50 values to crustaceans, mg/l	0.01 96 hr, Daphnia pulex (Govers et al. 1984)
Other information about water organisms	Lethal threshold concentration (LT50): Daphnia magna: 0.0018 mg/l, 0.52 days (Newsted & Giesy 1987) Pimephales promelas: 0.0018 mg/l, 2.71 days (Oris et al. 1987). Lepomis macrochirus, 1.0 mg/l, 6 hr, 87% mortality (Sax 1986).

233 • Benz[a]anthracene-7,12-quinone 2498-66-0

Sumformula of the chemical	C18H10O2	
Water solubility, mg/l	< 10	(MITI 1992)
Melting point, °C	168	(MITI 1992)
Log octanol/water coefficient, log Pow	4.4	(MITI 1992)
Total degradation in water	Biodegradation: 1% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	8.2–30 31–67	8w, Cyprinus carpio, conc 0.1 mg/l 8w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 100	48hr, Oryzias latipes (MITI 1992)

234 • Benz(b)anthracene 92-24-0

Sumformula of the chemical	C18H12	
Log octanol/water coefficient, log Pow	5.76	(Sangster 1989)
Other information about water organisms	Lethal threshold concentration (LT50): Daphnia magna: 0.68 days, 0.0006 mg/l (Newsted & Giesy 1987).	

235 • Benz(c)acridine 225-51-4

Synonyms	3,4-Benzacridine α-Chrysidine α-Naphthacridine 3,4-Benzoacridine	
Sumformula of the chemical	C17H11N	
Use	Occurs in engine exhaust gas at lower concentrations than polyaromatic hydrocarbons. Found in the atmosphere and in various air pollution emissions, including coal combustion stack effluent, petroleum refinery incinerator effluents, and coal tar pitch volatilised from coke plants.	
State and appearance	Insoluble yellow needles.	
Molecular weight	229.28	
Melting point, °C	108	
pKa	3.24	
Other physicochemical properties	Soluble in common organic solvents. Solubility in water may be enhanced by the presence of acids as impurities. Acridines are classified as weak bases.	
TDLo values to mammals in non-oral exposure, mg/kg	2400	skn-mus, 67W-I (Sax 1986)
Carcinogenicity	Repeated painting of benz(c)acridine solutions on the skin of mice and implantation of paraffin wax pellets containing benz(c)acridine into the bladders of rats produced tumors. Epitheliomas resulted from skin painting. The implantation in 58 rats induced 29 bladder papillomas, 8 of which were malignant, while only 2 rats implanted with control pellets developed benign papillomas. Not considered to be a highly active carcinogen. The lowest dose to induce a carcinogenic response in 468 mg/kg (Sax 1986).	
Mutagenicity	Mutagenic, mma, sat, 1 nmol/plate (Sax 1986).	
LC50 values to crustaceans, mg/l	0.45	24 hr, Daphnia pulex (Southworth et al. 1978)

236 • Benzaldehyde 100-52-7

Synonyms	Benzenecarbonal Oil of bitter almonds	
Sumformula of the chemical	C6H5CHO	
Odour	Characteristic: quality: bitter almonds.	
Molecular weight	106.13	
Specific gravity (water=1)	1.05	at 15/4 °C
Vapour density (air=1)	3.66	
Conversion factor, 1 ppm in air=	4.41	mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.227	ppm
Vapour pressure, mmHg	1 40	26 °C 90 °C
Water solubility, mg/l	3300 5000	 (MITI 1992)
Melting point, °C	-25	

Boiling point, °C	179 179 (MITI 1992)
Log octanol/water coefficient, log Pow	1.48 (Sangster 1989)
Total degradation in water	Biodegradation: 66% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	1300 orl-rat 28 orl-mus (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	5000 scu-rbt (Patty 1967)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): Bacteria (Pseudomonas putida): 132 mg/l (Bringmann & Kühn 1980a)
LC50 values to crustaceans, mg/l	> 15.8 96hr, Orconectes nais (Phipps & Holcombe 1985)
LC50 values to fishes, mg/l	11.2 96 hr, Salmo gairdneri, 1.07 96 hr, Lepomis macrochirus, 12.4 96hr, Pimephales promelas 13.8 96hr, Carassius auratus 5.39 96hr, Ictalurus punctatus (Phipps & Holcombe 1985) 1.269 4d, Salmo gairdneri (McKim et al. 1987)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): algae (Microcystis aeruginosa): 20 mg/l (Bringmann & Kühn 1976) green algae (Scenedesmus quadricauda): 34 mg/l protozoa (Entosiphon sulcatum): 0.29 mg/l (Bringmann & Kühn 1980a) protozoa (Uronema parduczi): 22 mg/l (Verschueren 1983) Fish: minnows: stop eating: 17.1 mg/l of 85% solution (McKee & Wolf 1963). Lethal threshold concentration (LT50): 3.79 mg/l, 0.8d (McKim et al. 1987). LC50, > 15,8 mg/l, 96hr, snail (Phipps & Holcombe 1985)

237• Benzanthrone 82-05-3

Use	Dyes.
State and appearance	Pale yellow needles.
Molecular weight	230.27
Water solubility, mg/l	< 10 (MITI 1992)
Melting point, °C	170 (MITI 1992)
Log octanol/water coefficient, log Pow	4.81 (MITI 1992)

Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	61–149 8w, Cyprinus carpio, conc 0.2 mg/l 79–181 8w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	> 100 48hr, Oryzias latipes (MITI 1992)
Other information about water organisms	Lethal threshold concentration (LT50): 0.0351 mg/l, 0.22 days; Daphnia magna (Newsted & Giesy 1987). Lethal threshold concentration (LT50): 0.0495 mg/l, 0.03 days; Pimephales promelas (Oris et al. 1987).

238 • Benzene

71-43-2

Synonyms	Benzol Coal naphta Phenyl hydride Cyclohexatriene
Sumformula of the chemical	C6H6
Use	Manufacturing styrene, phenol, detergents, organic chemicals, pesticide, plastics and resins, synthetic rubber, aviation fuel, pharmaceuticals, dye, explosives, PCB gasoline, tanning, flavors and perfumes, paints and coatings; nylon intermediates; food processing, photographic chemicals. As a solvent and a fuel additive; intermediate (25%); byproduct.
State and appearance	Colourless liquid.
Odour	Threshold Odour Concentration (T.O.C.): 0.516 mg/m³ = 0.160 ppm (Stockham et al. 1969) 43 mg/m³ = 13.3 ppm (Stockham et al. 1969) 1–300 ppm (Verschueren 1983) 4.68 ppm (Verschueren 1983) 1 ppm (Verschueren 1983) 60 ppm (Verschueren 1983, Summer 1971) 100 ppm (Verschueren 1983) 320 ppm (Verschueren 1983) 180 mg/m³ = 60 ppm (Verschueren 1983) 100.7 mg/m³ = 31.0 ppm (Verschueren 1983) 2.8 mg/m³ = 0.86 ppm (Verschueren 1983) recognition: 105–210 mg/m³ (Leonardos 1969) Population Identification Threshold 50%: 2.14 ppm Population Identification Threshold 100%: 4.68 ppm distinct odour: 310 mg/m³ = 90 ppm (Verschueren 1983). Human odour perception: 3.0 mg/m³ = 1 ppm Animal chronic exposure: adverse effect: 3.2 mg/m³ (Stern 1968). Threshold odour concentration in water: 2–31 mg/l (Fawell & Hunt 1988).
Molecular weight	78.12
Specific gravity (water=1)	0.8786 at 20/4 °C

Vapour density (air=1)	2.77
Conversion factor, 1 ppm in air=	3.26 mg/m³
Conversion factor, 1 mg/m³ in air=	0.31 ppm
Vapour pressure, mmHg	76 20 °C 95.19 25 °C (Boublik et al. 1984) 118 30 °C
Water solubility, mg/l	1791 (May 1980) 1769 25 °C (Aquan-Yuen et al. 1979) 1779.5 25 °C (Mackay & Shiu 1975) 700 (MITI 1992)
Melting point, °C	5.53 (Suntio et al. 1988)
Boiling point, °C	80.1 (MITI 1992)
Log octanol/water coefficient, log Pow	1.56–2.15 (Sabljic 1987) 2.13 (Anon. 1988) 2.11 (Schwarzenbach & Westall 1981) 1.56 (Hansch & Leo 1979) 2.15 (Hansch & Leo 1979) 2.39 (Veith et al. 1979) 2.12 (Banerjee et al. 1980) 2.2 (Hammers et al. 1982) 2.28 (Hanai et al. 1981) 2.16 (D'Amboise & Hanai 1982) 2.13 (Hansch & Leo 1985) 2.13 (Sangster 1989)
Log organic C/water coefficientlog Pcw	1.92 exptl (Schwarzenbach & Westall 1981) 1.98 exptl (Schwarzenbach & Westall 1981) 2.01 calcd (Schwarzenbach & Westall 1981)
Henry's law constant, Pa x m³/mol	430 (Anon. 1988) 562 exptl. (Mackay et al. 1979) 564 calc. (Yaws et al. 1991)
Volatilization	Relative volatility (nBuAc=1) = 6.91
Mobility	Equilibrium distribution: *mass %* air 99.34 water 0.65 solid 0.02 (Anon. 1988). Koc: Woodburn silt loam: 31 (Chiou et al. 1983) 31.7–143 (Sabljic 1984) 83 (Kenaga 1980). Benzene leaches in soil, passing through soil during bank infiltration (Green et al. 1981) (Piet & Morra 1983).

Photochemical degradation in air

Photochemical reaction; estimated lifetime under photochemical smog conditions in SE England: 28 hours (Verschueren 1983).

Gas-phase benzene will not be subject to direct photolysis but will react with photochemically produced hydroxyl radicals with a half-life of 13.4 days calculated using an experimental rate constant for the reaction. The reaction time in polluted atmospheres that contain nitrogen oxides or sulfur dioxide is accelerated with the half-life being reported as 4-6 hours with 50% mineralization to CO2 in approximately 2 days. Products of photo oxidation include phenol, nitrophenols, nitrobenzene, formic acid and peroxyacetal nitrate. (Korte & Klein 1982)

Since gas-phase benzene or benzene dissolved in cyclohexane does not absorb light of 290 nm or longer, it will not be expected to directly photolyze in sunlight in these media. However, slight shifts in wavelength of absorption might be expected in more representative environmental media, such as water; e.g., a half-life of 16.9 days was reported for photo lysis of benzene dissolved in deionized water saturated with air exposed to sunlight. (Howard & Durkin 1974) (Hustert et al. 1981)

Photochemical degradation in water

Photo degradation, which according to one experiment has a half-life of 17 days, could contribute to benzene's removal in situations of cold water, poor nutrients, or other conditions less conductive to microbial degradation. (Hustert et al. 1981)

Hydrolysis in water

Hydrolysis is not a significant process for benzene. (Lyman et al. 1982)

Chemical oxygen demand, g 02/g

2.15 5 days (Bridie et al. 1979)

Biochemical oxygen demand, g 02/g

2.18 5 days (Bridie et al. 1979)

Half-life in water, days

0.2	calculated, 25°, 1m depht (Verschueren 1983)
16	in river water
28	in ground water
	(Vaishnav & Babey 1987)

Aerobic degradation in water

Biodegradation to CO2 in estuarine water:

Conc. mg/l	*Month*	*Incubation time (hr)*	*Degradation rate (mg/l/day) x 1000*	*Turnover time (days)*
0.006	June	24	0.2	30
0.012	June	24	0.26	46
0.024	June	24	0.33	75

(Verschueren 1983).

Biodegradation half-lives of 28 and 16 days were reported in die-away for degradation of up to 3.2 µl/l benzene tests using ground water and Lester river water, respectively, under aerobic conditions. (Vaishav 1986)

Complete biodegradation in 16 days was reported under simulated aerobic ground water conditions at 20 °C. (Delfino & Miles 1985)

Total degradation in soil

If benzene is released to soil it will be subject to rapid volatilization near the surface, and which does not evaporate will be highly to very highly mobile in soil and may leach to the ground water. (Howard II 1990)

The effective half-lives for volatilization without water evaporation from soil to benzene uniformly distributed to 1 and 10 cm in soil were 7.2 and 38.4 days, respectively. (Jury et al. 1984)

Benzene may be subject to biodegradation based on reported biodegradation of 24% and 475 of the initial 20 ppm benzene in a base-rich para-brownish silt in 1 and 10 weeks, respectively. (Haider et al. 1974)

Total degradation in water

The estimated half-life for volatilization of benzene from a river 1 m deep flowing 1 m/sec with a wind velocity of 3 m/sec is estimated to be 2.7 hr at 20 °C. It will not be expected to significantly adsorb to sediment, bioconcentrate in aquatic organisms, or hydrolyse. It may be subject to biodegradation based on a reported biodegradation half-life of 16 days in an aerobic river die-away test. (Wakeham et al. 1983)

Biodegradation:
39–41% by BOD (on the upward trend)
period: 14d
substance: 100 mg/l
sludge: 30 mg/l
(MITI 1992).

Degradation and transformation products

phenol
unidentified phenols * using pure cultures of microorganisms (Smith & Rosazza 1974)

catecol
cis-1,2-dihydroxy-1,2-dihydrobenzene * using pure cultures of microorganisms (Gibson et al. 1968)

Ready biodegradability

Confirmed to be biodegradable (Anon. 1987).

Other information about degradation

ENVIRONMENT	*CONC. mg/l*	*REDOX-COND.*	*TEMP. °C*	*DEGRADATION %/day*	*REF.*
water	1–3	aerobic	20	100/16	a
water	1–3	anaerob	20	0/41	a
water	5	aerobic	25	49/7	b
water	10	aerobic	25	37/7	b
water (adapted)	5	aerobic	25	100/7	b
water (adapted)	10	aerobic	25	100/7	b
water	0.295	aerobic	-	92/17	c
groundwater	0.0041	aerobic	13	100/8	d
sludge	appr. 50	anaerob	35	0/56	e
sludge	appr. 50	anaerob	35	0/56	e
soil	0.613	methanogen	17	72/280	f
soil	0.613	methanogen	17	> 99/840	f
sterile soil	0.613	methanogen	17	0/280	f
sterile soil	0.613	methanogen	17	30/840	f

a) Delfino & Miles 1985
b) Tabak et al. 1981
c) Battermann 1984
d) Jamison et al. 1976
e) Horowitz et al. 1982
f) Wilson et al. 1986
(Anon. 1987b).

The half-life of benzene in estuarine water was 6 days. (Lee & Ryan 1979)

In a marine ecosystem biodegradation occurred in 2 days after an acclimation period of 2 days and 2 weeks in the summer and spring, respectively, whereas no degradation occurred in winter. (Wakeham et al. 1983)

Benzene at 50 ppm was 90% degraded by industrial wastewater seed incubated at 23 °C for 6 hours. (Davis et al. 1981)

B

Metabolism in mammals	No information appears to be available with regard to the gastrointestinal absorption of benzene, though a value of around 40–50% has been reported in several studies for respiratory absorption in humans. Percutaneous absorption has been demonstrated to occur slowly in man and rhesus monkey. Autoradiographic and pharmacokinetic studies have shown that benzene has an affinity for nervous and adipose tissue, with high levels also found in the bone marrow, liver, spleen and blood. Benzene is metabolized primarily in the liver to phenol, catechol, quinol and hydroxyquinol, and subsequently to conjugates of ester sulfates and glucuronides. In bone marrow, phenol appears to be the major metabolite shortly after exposure, though catechol and hydroquinone predominate subsequently. It is thought that secondary metabolites of the latter two compounds are probably responsible for the toxic effects of benzene in the bone marrow. The elimination of benzene by the lungs has been reported to be around 12% of the retained dose in humans but up to 70% in the experimental animals. Excretion in the urine as free or conjugated phenols accounts f by rodents (Fawell & Hunt 1988).
Bioconcentration factor, fishes	10.9 Clupea harengus pallasi, in eggs 6.9 Clupea harengus pallasi, yolk-sac larvae 3.9 Clupea harengus pallasi, feeding larvae (Verschueren 1983) 3.5 Anguilla japonica (Verschueren 1983) 3.5 Anquilla japonica (Ogata & Miyake 1978) 4.4 Clupea harengus pallasi (Korn et al. 1977) 4.3 Carassius auratus (Ogata et al. 1984)
Other information about bioaccumulation	Based on the reported and estimated BCF, benzene will not expected to bioconcentrate in aquatic organisms. (Howard II 1990)
LD50 values to mammals in oral exposure, mg/kg	3800 orl-rat (Sax 1984)
LCLo values to mammals in inhalation exposure, mg/kg	65 5 yr, ihl-hmn (Lewis & Sweet 1984)
TDLo values to mammals in oral exposure, mg/kg	130 orl-hmn (Lewis & Sweet 1984)
Effects on the physiology of mammals	Both epidemiological and animal studies have shown that pancytopenia is the most common effect of chronic exposure to benzene (Fawell & Hunt 1988).
Health effects	Man: severe toxic effects: 1500 ppm, 60 min symptoms of illness: 500 ppm unsatisfactory: 50 ppm (Verschueren 1983).
Carcinogenicity	There is good evidence that benzene can cause leukaemia in man, and some indication that it does also in experimental animals. This carcinogenic action of benzene also appears to be consistent with that of tumour promotion. There is no evidence of any other benzene-related tumours, apart from zymbal gland carcinomas and mammary carcinomas reported in one rat study (Fawell & Hunt 1988). Carcinogen (IARC).
Mutagenicity	Benzene has been reported to cause chromosomal abnormalities in vitro and in vivo in mammals, but has not yet been shown to be mutagenic in bacterial assays (Fawell & Hunt 1988).
Teratogenicity	Embryotoxicity through inhalation: CF-1 mice and New Zealand white rabbits were exposed to 0 or 500 ppm of benzene fo 7 hr per day from days 6 through 15 (mice) and 6 through 18 (rabbits) of gestation. Little evidence of maternal toxicity was seen in either species. Although some signs of embryonal toxicity were observed in both mice and rabbits, a teratogenic effect was not discerned in either species inhaling 500 ppm of benzene (Verschueren 1983). Benzene can cause retardation of foetal development at high doses, but does not appear to be teratogenic (Fawell & Hunt 1988).

Effects on amphibia	Mexican axoloth (3–4 weeks after hatching): LC50 48 hr: 370 mg/l; clawed toad (3–4 weeks after hatching): LC50 48 hr: 190 mg/l (Slooff & Baerselman 1980).	
Maximum longterm immission concentration in air for plants,mg/m³	3	VDI 2306
Maximum longterm immission concentration in air for plants,ppm	1	VDI 2306
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 92 mg/l (Bringmann & Kühn 1980a).	
EC50 values to microorganism, mg/l	1500 50 > 150	15 min Microtox (Hermens et al. 1985) Microtox (Vasseur et al. 1986) Microtox 20 °C (Vasseur et al. 1986)
EC50 values to algae, mg/l	29	growth, 3d, Selenastrum capricornutum (Galassi et al. 1988)
NOEC values to algae, mg/l	600	Selenastrum capricornutum (Slooff et al. 1983)
LC50 values to crustaceans, mg/l	15	96 hr, Daphnia pulex (Govers et al. 1984)
	27	96 hr, Palaemonetes pugio (Neff et al.1976)
	108	96 hr, Cancer magister, crab larvae-stage 1
	20	96 hr, Crangon franciscorum (Verschueren 1983)
	305 430 370	48 hr, Daphnia pulex 48 hr, Daphnia magna 48 hr, Daphnia cucullata (Canton & Adema 1978)
	120 42	48 hr, Asellus aquaticus (Slooff 1983) 48 hr, Gammarus pulex (Slooff 1983)
EC50 values to crustaceans, mg/l	18	24hr, Daphnia magna (Galassi et al. 1988)
LC50 values to fishes, mg/l	5.3 15.1	96 hr, Salmo gairdneri 96hr, Pimephales promelas 1982 (DeGraeve et al.)
	0.015 0.025	96 hr, Thymallus arcticus 96hr, Gasterosteus aculeatus (Moles et al. 1979)
	20	48hr, Lepomis macrochirus (McKee & Wolf 1963)
	5.8–10.9	Morone saxatilis (Verschueren 1983)
	12	1hr, Salmo trutta m. lacustris (Woodiwiss & Fretwell 1974)
	56	48hr, Salmo gairdneri (Slooff et al.1983)
	46	24hr, Carassius auratus (Bridie et al.1979)
	64	16 days, Poecilia reticulata (Hermens et al. 1985)
	9.2 425 102–910 100–600	24hr, 96hr, Salmo gairdneri 24hr, 96hr, Ictalurus punctatus 24hr, Lepomis macrochirus 96hr, Lepomis macrochirus (Mayer & Ellersieck 1986)
	28.6 5.9	4d, Poecilia reticulata 4d, Salmo gairdneri (Galassi et al. 1988)

Effects on the reproduction of water organisms	Herring and anchovy larvae (Clupea pallasi; Engraulis mordex): 35–45 ppm caused delay in development of eggs and produces abnormal larvae; 10–35 ppm caused delay in development of larvae; decrease in feeding and growth, and increase in respiration (Verschueren 1983).
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): algae (Microcystis aeruginosa): > 1400 mg/l (Bringmann & Kühn 1976) green algae (Scenedesmus quadricauda): > 1400 mg/l protozoa (Entosiphon sulcatum): > 700 mg/l protozoa (Uronema parduczi): 486 mg/l (Bringmann & Kühn 1980) Chlorella vulgaris: 50% reduction of cell numbers vs controls, after 1 day incubation at 20 °C: at 525 ppm (Verschueren 1983). Inhibition of photosynthesis of a freshwater, non axenic uni-algal culture of Selenastrum capricornutum: 10 mg/l: 95% carbon-14 fixation (vs. controls) 100 mg/l: 84% carbon-14 fixation (vs. controls) 1000 mg/l: 5% carbon-14 fixation (vs. controls) (Verschueren 1983). Ciliate (Tetrahymena pyriformis): 24 hr LC100: 12.8 mmol/l (Schultz et al. 1978). Minnows: min. lethal dose: 5–7 mg/l; 6 hr (McKee & Wolf 1963). Young Coho salmon: no significant mortalities up to 10 ppm after 96 hours in artificial sea water at 8 °C; mortality: 12/20 at 50 ppm after 24 up to 96 hours in artificial sea water at 8 °C; mortality 30/30 at 100 ppm after 24 hours in artificial sea water at 8 °C (Verschueren 1983). LC50, 48hr, > 320 mg/l, Tubificidae LC50, 48hr, 100 mg/l, Chironomus gr. thummi LC50, 48hr, > 320 mg/l, Erpobdella octoculata LC50, 48hr, 230 mg/l, Lymnaea stagnalis LC50, 48hr, 74 mg/l, Dugesia cf. lugubris LC50, 48hr, 34 mg/l, Hydra oligactis LC50, 48hr, 48 mg/l, Corixa punctata LC50, 48hr, 10 mg/l, Ischura elegans LC50, 48hr, 130 mg/l, Nemoura cinerea LC50, 48hr, 34 mg/l, Cloeon dipterum (Slooff 1983)
Other information	Manufacturing source: petroleum refinery; solvent recovery plant; coal tar distillation; coal processing; coal coking (Anon. 1975). The major source of atmospheric benzene is vehicle echausts. Benzene is found in many foodstuffs and beverages at significant levels. Exposure to waterborne benzene at current levels is almost insignificant in comparison to exposure from other sources (Fawell & Hunt 1988).

239 • Benzenesulfochloride 98-09-9

Synonyms	Benzenesulfonylchloride Benzenesulfonchloride
Use	Dye manufacturing (intermediate); accelerator in alkyl resin formation; phenol manufacturing (intermediate); manufacturing resorcinal (intermediate).
Molecular weight	176.62
Specific gravity (water=1)	1.378 at 23 °C
Melting point, °C	14.5

Degradation point, °C	246	
LC50 values to fishes	3	48 hr, Salmo trutta yearlings (Verschueren 1983)

240 • Benzenesulfoneamide
98-10-2

Water solubility, mg/l	> 10000	(MITI 1992)
Melting point, °C	156	(MITI 1992)
Log octanol/water coefficient, log Pow	0.31	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.39–1.2 < 3.8–5.8	6w, Cyprinus carpio, conc 2 mg/l 6w, Cyprinus carpio (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	440	48hr, Oryzias latipes (MITI 1992)

241 • Benzenesulfonic acid
98-11-3

Molecular weight	158.17	
Log octanol/water coefficient, log Pow	-2.25	calculated
Total degradation in water	Biodegradation: 87% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
Other information about degradation	Biodegradation: decomposition by a soil microflora: 16 days (Verschueren 1983).	
LD50 values to mammals in oral exposure, mg/kg	400–3200	orl-mus (Patty 1967)
Health effects	Man: severe skin irritation (Patty 1967).	
LD50 values to birds in oral exposure, mg/kg	> 100 75	orl-Agelaius phoeniceus orl-Sturnus vulgaris (Schafer et al. 1983)

242 • Benzethonium chloride
121-54-0

Sumformula of the chemical	C27H42ClNO2H2O
Use	Pesticide; antiseptic; cationic detergent.

State and appearance	Colourless, odourless plates, very bitter taste.	
Odour	Odourless.	
Molecular weight	466.1	
Melting point, °C	164–166	
Other information about degradation	Biodegradation: at 18 mg/l no degradation after 28 days by nonadapted sewage (Verschueren 1983).	
Health effects	Man: highly toxic by ingestion; 1 gram may be fatal (Verschueren 1983).	
Effects on microorganisms	Bacteria: Staphylococcus aureus: at 20 mg/l bacteriolytic action after 1 hour; bacteria isolated from Phone (France) water: at 20 mg/l no significant reduction of growth rate (Verschueren 1983).	
LC50 values to crustaceans, mg/l	70	96hr, Penaeus californiensis (Hanks 1976)
LC50 values to fishes, mg/l	1.6 1.4 53	96hr, Pimephales promelas 96hr, Lepomis macrochirus (Surber & Pickering 1962) 96hr, Oncorhynchus kisutch (Verschueren 1983)

243 • Benzidine 92-87-5

Synonyms	p, p'-Bianiline 4,4'-Diaminobiphenyl	
Sumformula of the chemical	C12H12N2	
Use	Organic synthesis; manufacture of dyes.	
State and appearance	Grayish-yellow, white or reddish gray crystalline powder.	
Molecular weight	184.23	
Specific gravity (water=1)	1.25	at 20/4 °C
Vapour density (air=1)	6.36	
Density, kg/m³	1250	20 °C
Water solubility, mg/l	400 9400	at 12 °C at 100 °C
Melting point, °C	116–129	
Boiling point, °C	402	
Log octanol/water coefficient, log Pow	1.37 1.81	(Anon. 1989)
Mobility	Theoretical distribution: > 91% in water, the rest in sediment and soil (Nordic 1988).	
Other reactions in atmosphere	Probable reactions in air: photo lysis and oxidation with ozone. Estimated half-life approximately 1 day (Radding et al. 1975).	
Total degradation in soil	80% reduction after 4 weeks incubation in soil (Lu et al. 1977). Degradation ways: methylation, acetylation in microbial degradation in soil (Lu et al. 1977).	
Total degradation in water	Degradation in soil - enzymes, photochemical, free radicals. Half-life in water: approximately 100 days (Radding 1975).	

Other information about degradation	Possible biooxidation products scanned by GC/MS: N-hydroxybenzidine; 3-hydroxybenzidine; 4-amino-4'-nitrobiphenyl; N,N'-dihydroxybenzidine; 3,3'-dihydroxybenzidine; 4,4'-dinitrobiphenyl (Verschueren 1983). Not easily degradable (Rudoph & Boje 1988). Benzidinedihydrochloride is more persistent than benzidine (Bowman et al. 1976). Activated, aerated active sludge promotes degradation of benzidine (Tabak & Barth 1978). 85–93% reduction of 20 mg/l benzidine after 6 hours at 20 °C in biological aerobic wastewater treatment process (Baird et al. 1977). Degradation products of special interest: Acetyle derivate of benzidine (microbial degradation, metabolites); colouring agents based on benzidine degrade to benzidine; with chlorination of benzidine in water forms degradation products of chloroamine type (IARC 1982, Lu et al. 1977, Jenkins & Baird 1975).
Other information about metabolism	Fastly absorbed (USEPA 1980d). 3-hydroxybenzidine (80–90%), diacetylbenzidine (5–10%), monoacetylbenzidine (1–5%) and benzidine is detected in urine (IARC 1982).
Bioconcentration factor, fishes	55 Gambusia (Lu et al. 1977) 38–44 Lepomis, 42d (EG & Bionomics 1975)
Bioconcentration factor, crustaceans	290 Daphnia (Lu et al. 1977)
Bioconcentration factor, algae	2620 Oedogonium (Lu et al. 1977)
Bioconcentration factor, other organisms	650 Physa (Lu et al. 1977)
LD50 values to mammals in oral exposure, mg/kg	1570 orl-rat (Marhold et al. 1968)
Carcinogenicity	Carcinogenicity: positive (McCann et al. 1975). Colouring agents based on benzidine induces cancer in rats and people, at the same time as benzidine is detected in urine (IARC 1982). Acetyle derivate of benzidine induces cancer in test animals and are mutagen in Ames test with metabolic activation (IARC 1982).
Mutagenicity	Mutagenicity in the Salmonella test: positive; 1.4 revertant colonies/nmol 265 revertant colonies at 0.050 mg/plate (McCann et al. 1975). Mutagen in Ames test when metabolic activation is present (Fishbein 1984). Mutagenic effects in Drosophila melanogaster (Fahmy & Fahmy 1977). Chromosome changes in people exposed at work (Bassendowska-Karska 1980).
LC50 values to crustaceans, mg/l	> 20 96hr, Gammarus (USEPA 1980d)
EC50 values to crustaceans, mg/l	1.1 24hr, Daphnia (Rudolph & Boje 1988)
LOEC values to crustaceans, mg/l	0.1 21d, Daphnia (Rudolph & Boje 1988)
NOEC values to crustaceans, mg/l	0.032 21d, Daphnia (Rudolph & Boje 1988)

LC50 values to fishes, mg/l	92	96hr, Leuciscus (Rudolph & Boje 1988)
	> 20	96hr, Pimephales (USEPA 1977)
	7.4	96hr, Salmo gaidneri
	4.35	Salvelinus namaycush
	2.5	Notropis lutrensis
	16.2	Jordanelia floridae (USEPA 1980d)
Effects on the physiology of water organisms	Ctenopharyngodon idella; Cyprinus carpio; Tinca tinca: 10 mg/kg, 2 days; cytogenetic effect: changes in the RNA and DNA of the cell) (Al-Sabti 1986).	

244 • Benzidine dihydrochloride 531-85-1

Other information about degradation	Impact on biodegradation: NH3 oxidation by Nitrosomonas sp. at 100 mg/l: 84% inhibition at 50 mg/l: 56% inhibition at 10 mg/l: 12% inhibition (Hockenbury & Grady 1977).

245 • Benzo(a)fluorene 238-84-6

Sumformula of the chemical	C17H12
Molecular weight	216.28
Melting point, °C	187–189
Boiling point, °C	407
Log octanol/water coefficient, log Pow	5.4 (Sangster 1989)
Other information about water organisms	Lethal threshold concentration (LT50): Daphnia magna; 0.0048 mg/l, 0.96 days (Newsted & Giesy 1987).

246 • Benzo(a)pyrene 50-32-8

Synonyms	3,4-Benzopyrene B(a)P Benz(a)pyrene 1,2-Benzpyrene Benzo(def)chrysene 6,7-Benzopyrene
Sumformula of the chemical	C20H12
Use	Benzo(a)pyrene is found in coal tar, cigarette smoke, and in the atmosphere as a product of incomplete combustion. It is found in the exhaust soot and tar from gasoline and diesel engines. It is also found in oil, water, and food. Used in cancer research.
State and appearance	Pale yellow plates or long needles. Monoclinic or orthorhombic crystals. Practically insoluble.
Molecular weight	252.3
Vapour pressure, mmHg	0.0000000055, 25 °C
Water solubility, mg/l	0.005–0.010 in seawater at 22 °C

Melting point, °C	179	
Boiling point, °C	311	at 10 mm
Log octanol/water coefficient, log Pow	7.23 6.35	calculated (Anon. 1989) (Sangster 1989)
Volatilization	Adsorption on and movement via the sediment is probably a more important transport process than volatilization. – The half-life for benzo(a)pyrene volatilization was 1500 hr, calculated for a river 1 m deep, water velocity 0.5 m/second, and wind velocity 1m/second (Sax 1986).	
Adsorption/desorption	Adsorption: in estuarine water; at 0.003 mg/l, 71% adsorbed on particles after 3 hours (Lee 1977). A one-compartment model that simulated river conditions, predicted that 83% or the benzo(a)pyrene would be sorbed onto suspended solids. The same model predicted 71% sorption in eutrophic and oligotrophic lakes and 93% in eutrophic ponds. The half-life of all fate processes combined including dilution according to this model ranged from 0.48 hr in a stream to 7.4 hr in an eutrophic lake. The percentage of sorbed B(a)P in various surface waters and wastewaters was 24–44% at 22 °C. The log of the mean partition coefficient between the suspended particulates and the water was 4.48 (Sax 1986).	
Other bindings	After 3 hours incubation in natural seawater, 75% of 0.002 mg/l were taken up by suspended aggregates of dead phytoplankton cells and bacteria (Lee et al. 1978).	
Other physicochemical properties	Insoluble.	
Photochemical degradation in air	The most common photooxidation product of PAHs in solution in an endo peroxide. Dealkylation, ring cleavage, and other reactions ensue following photolysis or pyrolysis of these peroxides. Frequently, only quinones are isolable. Photodimers may result in some cases. Adsorbed PAHs are more reactive than in solution (Sax 1986). Ozone and UV irradiation degraded more than half of the pure benzo(a)pyrene present in a simulated atmosphere after 0.50 hours. However, photooxidation in the atmosphere is not as rapid as predicted from model laboratory studies. Detectable levels of PAHs are usually found in urban atmospheres. – Benzo(a)pyrene in simulated atmospheres containing 1 ppm nitrogen dioxide and approximately 10 ppb nitric acid formed nitro derivatives that were directly mutagenic in the Ames test (Sax 1986).	
Other reactions in atmosphere	Airborne particulate PAHs can persist at relatively high concentrations in aerosols transported for long distances. The atmosperic persistence is longer than would be predicted from laboratory photo oxidation studies. On the other hand, The National Academy of Sciences (1972) proposed that the chemical half-life of PAH's in the atmosphere may be limited to hours or days. For example, the half-life for benzo(a)pyrene with ozone in the gas phase is 870 hours (Sax 1986).	
Photochemical degradation in water	The half-life for photo lysis calculated for surface waters in midsummer at 40° N latitude is 0.54hr. B(a)P photo oxidation in natural waters depends on water depth and varies seasonally due to changes in solar radiation, temperature and dissolved oxygen. Because or the lack of solar radiation and oxygen, photo oxidation in sediments is negligible (Sax 1986).	
Hydrolysis in water	PAHs do not contain groups amenable to hydrolysis (Sax 1986).	

Oxidation-reduction reactions	Ozone and chlorinating agents oxidize polycyclic aromatic hydrocarbons to quinones, diacids, and nuclear and side-chain oxidation products. Chlorinating agents also produce chlorine-substituted derivatives. – Oxidation of any PAH by chlorine and ozone, when used for the disinfection of drinking water, forms quinones. The half-life for the reaction of chlorine with all PAHs is less than 0.5 hr (Sax 1986). Oxidation by chromic acid or ozone gives benzo(a)pyrene-1,6-quinone and benzo(a)pyrene-3,6-quinone. Further oxidation gives benzanthrone dicarboxylic anhydride (Sax 1986). Oxidation of any PAH by chlorine and ozone, when used for the disinfection of drinking water, forms quinones. – Chlorinating agents will also produce chlorine-substituted PAHs as well as oxidation products. – The half-life of benzo(a)pyrene in the presence of ozone is approximately 1 hour and in the presence of 0.5 ppm chlorine, 10 minutes (Sax 1986). Oxidation by RO2 radical is slow and not significant with a half-life of 96 hr. The dissolved portion may undergo rapid photolysis with a half-life of 1–2 hours (Sax 1986).
Aerobic degradation in water	Microbial degradation to CO2 in seawater at 12 °C in the dark after 48 hr incubation at 0.016 mg/l: 0 μg/l/day; after addition of water extract of fuel oil 2, after 24 hr incubation: 0.00001 mg/l/day – turnover time: 1400 days (Verschueren 1983). Biodegradation to CO2 in estuarine water:

conc. mg/l	*month*	*incubation time (hr)*	*degradation rate (mg/l/day) x 1000*	*turnover time (days)*
0.005	January	24	0	-
0.005	June	24	0	-
0.005	May	96	0.002	3500

(Lee 1977).

Degradation in seawater by oil oxidizing microorganisms (in presence of 0.365 mg/l pyrene and 0.35 mg/l fluorene at 10 °C): initial conc. 0.190 mg/l; after 12 days: 0.090 mg/l: 53% decrease (McKenzie & Hughes 1976).

Total degradation in soil	Soil systems provide better conditions for biodegradation than do aquatic systems. The rate and degree of degradation is greatest when the soil and its microbial population has been acclimated. – Mycobacterium rubrom and M. flavum metabolized approximately half or the compound within 4 days. – Strains of bacteria from highly contaminated soil could metabolize 75–86 % or the B(a)P within 5 days, Bacteria from less contaminated soil metabolized 48–59% within the same time period. – It has been claimed that soil microorganims decompose B(a)P when present at high concentrations (30 ppm), but that B(a)P is not readily degraded when concentrations are lower (Sax 1986). Degradation is soil: 82% after 8 days (soil + adapted bacteria) (Lee & Takahashi 1977).
Total degradation in water	Biological degradation in sea water (10 °C): 53% after 12 days (McKenzie & Hughes 1976).
Total degradation in sediment	PAHs deposited in sediments are less subject to photochemical or biological oxidation, especially if the sediment is anoxic. Sedimentary PAH is therefore quite persistent and may accumulate to high concentrations (Sax 1986).

Other information about degradation

Average degradation by soil bacteria after 8 days culture:

	amount of extracted B(a)P mg	*amount of B(A)P destroyed (%)*
soil not inoculated with bacteria (control)	0.191	0
soil + N 5 bacterial strain	0.090	53
soil + N 13 bacterial strain	0.061	66
soil + N 13 bacterial strain*	0.033	82

*before the experiment this strain was cultured in a medium containing B(a)P for 110 days (Poglazova et al. 1967).

Degradation of benz(a)pyrene:

ENVIRONMENT	*CONC. mg/l*	*REDOX-COND.*	*TEMP. °C*	*DEGRADATION %/day*	*REF.*
sediment	1.25	aerobic	30	6.3/37	a
sediment	1.25	anaerob	30	0.09/37	a
sediment	7	aerobic	-	0/1	b
sediment	17	aerobic	20	0.84/7	c
sand	7.6	aerobic	20	1.4/7	c
sand	9.5	aerobic	20	1.2/7	c
soil	1	aerobic	-	13/25	d
soil	5	aerobic	-	6/25	d
soil	10	aerobic	-	3/25	d
soil (adapted)	1	aerobic	-	23/25	d
soil (adapted)	2.5	aerobic	-	20/25	d
soil (adapted)	5	aerobic	-	30/25	d
soil (adapted)	10	aerobic	-	10/25	d
soil	9.5	aerobic	-	33/90	e
soil	545	aerobic	-	71/90	e
soil (adapted)	28.5	aerobic	-	52/90	e
soil	0.06	aerobic	28	66/8	f
soil	0.09	aerobic	28	53/8	f
soil (adapted)	0.09	aerobic	28	82/8	f

a) Delaune et al. 1981
b) Herbes 1981
c) Gardner et al. 1979
d) Löw 1983
e) Khesina et al. 1969
f) Poglazowa et al. 1967

(Anon. 1987b).

Above-ground parts of plants contain more B(a)P than underground parts. The concentration is directly proportional to exposure time during the growing season and surface area of the plant (Sax 1986).

Other information about metabolism

There are large differences among aquatic species in their ability to absorb and assimilate PAH from food. Polychaete worms have a very limited ability; fish show limited and variable absorption from the gut; and crustaceans readily assimilate PAH. Assimilated PAHs are metabolized and excreted rapidly. For biomagnification to occur, a substance must be relatively resistant to metabolism or exretion (Sax 1986).

Callinectes sapidus, half-life < 2 days (Lee 1976).

Half-life in Mytilus: 16 days (Knutzen & Skei 1988).

B(a)P is metabolized to approximately 20 primarily and secundarily oxidized metabolites and many conjugates. Many metabolites induces mutagenicity, cell alterations and/or binds to cellular macromolecules (IARC 1984).

Bioconcentration factor, fishes

70.7 7 d, Salmo salar (Verschueren 1983)

B

Bioconcentration factor, mollusca	190 3000 861 8.7	2 days, Crassostrea virginica 8 days, Crassostrea virginica (Lee et al. 1978) Macoma inquinata, 7d Rangia cuneata, 24hr (Sax 1986)
Bioconcentration factor, crustaceans	242	2d, Callinectes sapidus (Lee 1976)
Bioconcentration factor, other organisms	28200	aquatic organisms containing 7.6% lipids, estimated (Sax 1986)
LD50 values to mammals in non-oral exposure, mg/kg	50	scu-rat (Lewis & Sweet 1984)
LDLo values to mammals in non-oral exposure, mg/kg	500	ipr-mus (Sax 1986)
TDLo values to mammals in oral exposure, mg/kg	40 100 1600 160 700	orl-rat, 14d preg, teratogenic orl-mus, 7-16d preg, teratogenic orl-mus, 7-16d preg, teratogenic orl-rat, 6D-C, tumorigenic orl-mus, 75W-I, tumorigenic (Sax 1986)
TDLo values to mammals in non-oral exposure, mg/kg	60 150 10 160 10 17	ipr-rat, 16-18d preg, teratogenic ipr-mus, 8d preg, teratogenic ipr-ham, 5d male, teratogenic scu-mus, tumorigenic ivn-mus, tumorigenic skn-rbt, 57W-I, tumorigenic (Sax 1986)
TCLo values to mammals in inhalation exposure, mg/kg	9.5	ihl-ham, 4hr, 96W-I, tumorigenic (Sax 1986)
Effects on the physiology of mammals	Besides producing malignant tumors in laboratory animals, benzo(a)pyrene damages the lymphoid system, induces tracheobronchial epithelial proliferation and cell hyperplasia without necrosis or inflammation, and suppresses the immune system. Dosed rodents show tissue destruction in the pancreas and liver, and abnormal sperm (Sax 1986).	
Health effects	PAHs can presumably be absorbed from ingestion, inhalation and skin contact (Sax 1986). Skin and eye irritation data: skn, mus, 0.014 mg, mild (Sax 1986).	
Carcinogenicity	Carcinogenicity: positive (McCann et al. 1975). Strongly carcinogenic. B(a)P is a complete carcinogen, providing both initiating and promoting stimuli. – Benzo(a)pyrene produced tumours in all of the animal species for which data were reported in 1973. Different administration included oral, skin, and intratracheal routes. Its carcinogenic effect is both local and systemic. It produced local sarcomas in subhuman primates after repeated subcutaneous injections and lung carconomas after intratracheal instillation. In addition, it initiated skin carcinogenesis in mice and proved carcinogenic after single doses and prenatal exposure. – B(a)P has also induced tumours in salivary glands, pancreas, subcutaneous tissues, mammary grands, uterus, vagina, kidney, brain, and thymus (Sax 1986).	

Mutagenicity	Mutagenicity in the Salmonella test: positive; 121 revertant colonies/nmol 2398 revertant colonies at 0.005 mg/plate (McCann et al. 1975). Mutagenicity: induced significant mutation to 8-azaguanine resistance in Salmonella typhimurium at concentrations as low as 0.004 mM (Krishnan et al. 1979). Mutagenic to mice and bacteria. Cell cultures of many species including man show inhibition of DNA synthesis after treatment with B(a)P. – Certain metabolites of B(a)P, especially the diol epoxides, are much more mutagenic in Salmonella typhimurium TA98 and chinese hamster V79 cells than B(a)P itself. – B(A)P was found to be positive in the sister chromatid exchange test, weakly active in the chromosome aberration test, and negative in the micronucleus test (Sax 1986). Mutagen data: mmo, sat, 0.333 mg/plate; mrc, esc, 0.070/well; dnr, ocs, 0.100 ml/plate; dnd, omi, 11 ng/l; dnd, sal, tes, 0.005, 1 H-C; msc, ofs, fbr, 5 mg/l; dnd, hmn, oth, 1500 nmol/l; dnd, hmn, lng, 0.001 mmol/l (Sax 1986).
Effects on wastewater treatment	Polychlorinated PAHs are probably highly toxic to aquatic organisms and persistent in the environment as are polychlorinated biphenyls and polychlorinated naphthalenes. Chlorination for purification of wastewaters or drinking waters containing high concentrations of PAHs may be inadvisable. Activated sludge treatment is unable to oxidize PAHs within normal retention times. Since large PAHs are insoluble in water, either they do not support bacterial growth or growth may be extremely slow. The problem has been somewhat overcome by use of other carbon sources to stimulate (or induce) bacteria. Apparently, long-term exposure of microbes is necessary before a bacterial population is capable of degrading PAHs (Sax 1986).
EC50 values to algae, mg/l	> 4 3d, grw, Anabaena flos-aquae > 4 3d, grw, Chlamydomonas reinhardtii > 4 3d, grw, Euglena gracilis 0.005 3d, grw, Scenedesmus obliquus 0.015 3d, grw, Selenastrum capricornutum > 4 3d, grw, Poteriochromonas malhamensis (Schoeny et al. 1988)
LC50 values to crustaceans, mg/l	0.05 96 hr, Daphnia pulex (Govers et al. 1984)
Effects on the physiology of water organisms	Ctenopharyngodon idella; Cyprinus carpio; Tinca tinca: 10 mg/kg, 2 days, cytogenetic effect (changes in the RNA and DNA of the cell) (Al-Sabti 1986). Lepomis macrochirus; 0.005 mg/g, 3 days, biochemical effect (change in physiochemical process including glycogen uptake, cholesterol levels and lipid analysis) (Shugart et al. 1987). Salmo gairdneri; 0.63 mmol, 6 days, biochemical effect (change in physiochemical process including glycogen uptake, cholesterol levels and lipid analysis) (Miyauchi & Uematsu 1987). Ictalurus nebulosus; 4 d, 0.005–0.025 mg/g, cytogenetic effect (Metcalfe 1988). Lepomis macrochirus, 10 d, 0.001–0.020 mg/g, enzyme effect (Jimenez & Burtis 1988). Poeciliopsis monacha, 1 d, 0.8–1.0 mg/l, enzyme effect; Poeciliopsis sp, 1 d, 3.75 mg/l, lethal effect (Goddard et al. 1987).

B

Other information about water organisms	Lethal threshold concentration (LT50): Daphnia magna; 0.0015 mg/l, 0.19 days (Newsted & Giesy 1987) Pimephales promelas; 0.0056 mg/l, 1.67 days (Oris et al. 1987). Acute toxicity to fish: High molecular PAH (B(a)P, chrysene) have generally low acute toxicity, probably due to their low solubility (Neff 1979). Chronic toxicity: Chronic toxicity (carcinogenicity, mutagenicity, teratogenicity) is a concequence of high activated, soluble metabolites of B(a)P via covalent bindning to cellular macromoleculs (Heidelberger 1976). The growth of algae is stimulized by low concentrations of B(a)P (0.01–0.1 mg/l) (Graf & Nowak 1966, Boney & Corner 1962).
Other information	Manufacturing source: coal tar processing; petroleum refining; shale refining; coal and coke processing kerosene processing; heat and power generation sources. Natural sources: quantities synthesized by various bacteria: *mg of B(a)P produced* *per kg of species* — *dry bacterial biomass* Mycobacterium smegmatis — 0.060 Proteus vulgaris — 0.056 Escherichia coli (strain 1) — 0.050 Escherichia coli (strain 2) — 0.046 Pseudomonas fluorescens — 0.030 Serratia marcescens — 0.020 Synthesized by algae Chlorella vulgaris. Man caused sources (air and water): combustion of tobacco, combustion of fuels; present in run off containing greases, oils, etc.; potential roadbed and asphalt leachate. (Verschueren 1983) > 10% of to atmosphere emitted B(a)P goes to water environment (Neff 1979). Microbial degradation to 9-hydroxybenzo(a)pyrene and acids (Gibson 1976b). Degradation products with special interest: benzo(a)pyrenequinones; 9,10-epoxy-7,8-dihydrozybenzo(a)pyrene; B(a)P-dihydrodioles; B(a)P-diolepoxides; B(a)P-oxides (USEPA 1980).

247 • Benzo-α-pyrone — 91-64-5

Synonyms	Coumarin 1,2-Benzopyrone o-Coumaric acid lactone Coumarinic lactone Cumarin Tonka bean camphor	
State and appearance	Colourless crystals, flakes or powder.	
Odour	Quality: vanilla Hedonic tone: pleasant	
Molecular weight	146.14	
Specific gravity (water=1)	0.935	at 20/4 °C
Vapour pressure, mmHg	1 40	at 106 °C at 189 °C
Water solubility, mg/l	100	at 25 °C
Melting point, °C	68	(MITI 1992)

Boiling point, °C	291 (MITI 1992)
Log octanol/water coefficient, log Pow	1.39
Total degradation in water	Biodegradation: 100% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	235–290 orl-rat (Verschrueren 1983)

248 • Benzo(b)fluoranthene 205-99-2

Synonyms	3,4-Benzfluoranthene B(b)F
Sumformula of the chemical	C20H12
Molecular weight	252
Log octanol/water coefficient, log Pow	5.78 (Sangster 1989)

249 • Benzo(b)fluorene 30777-19-6

Molecular weight	216.28
Melting point, °C	209–210.5
Other information about water organisms	Lethal threshold concentration (LT50): Daphnia magna: 0.0022 mg/l, 0.93 days (Newsted & Giesy 1987).

250 • Benzo(e)pyrene 192-97-2

Synonyms	1,2-Benzopyrene B(e)P
Molecular weight	252
Water solubility, mg/l	0.004 at 25 °C
Carcinogenicity	Carcinogenicity: weakly carcinogenic (McCann et al. 1975).
Mutagenicity	Mutagenicity in the Salmonella test: positive; > 60 revertant colonies/nmol 143 revertant colonies at 0.060 mg/plate (McCann et al. 1975).
Other information about water organisms	Lethal threshold concentration (LT50): Daphnia magna: 0.0007 mg/l, 0.64 days (Newsted & Giesy 1987).

251 • Benzo(ghi)perylene 191-24-2

Synonyms	1,12-Benzoperylene B(ghi)P

B

Sumformula of the chemical	C22H12
Use	Main constituent in the residues from coal hydrogenation.
State and appearance	Large pale yellow-green plates.
Molecular weight	276.34
Vapour pressure, mmHg	0.0000000001
Water solubility, mg/l	0.00026 at 25 °C
Melting point, °C	222 273
Log octanol/water coefficient, log Pow	7.23 (Sax 1986) 6.51 (Sax 1986) 6.9 (Sangster 1989)
Volatilization	Evaporation of lower-molecular-weight PAHs may be significant only in a clear, rapidly flowing shallow stream (Sax 1986).
Adsorption/desorption	Movement via sediment is an important transport process. An exchange equilibrium exists in natural water systems between absorbed and soluble PAHs. Although the particulate form is favoured, a significant fraction of the PAH will be dissolved except in systems that are very heavily contaminated by PAHs (Sax 1986).
Other physicochemical properties	Insoluble.
Photochemical degradation in air	The most common photooxidation product of PAHs in solution in an endo peroxide. Dealkylation, ring cleavage, and other reactions ensue following photo lysis or pyrolysis of these peroxides. Frequently, only quinones are isolable. Photo dimers may result in some cases. Adsorbed PAHs are more reactive than in solution (Sax 1986).
Photochemical degradation in water	Photo lysis in an aquatic environment may be an important fate process, especially for the dissolved portion (Sax 1986).
Hydrolysis in water	Hydrolysis is not significant (Sax 1986).
Oxidation-reduction reactions	Ozone and chlorinating agents oxidize polycyclic aromatic hydrocarbons to quinones, diacids, and nuclear and side-chain oxidation products. Chlorinating agents also produce chlorine-substituted derivatives. – Oxidation of any PAH by chlorine and ozone, when used for the disinfection of drinking water, forms quinones. The half-life for the reaction of chlorine with all PAHs is less than 0.5 hr. – Treating benzo(ghi)perylene with 2.2 ppm free chlorine at 20° C and pH 6.8 for 15 minutes reduced its concentration by 50%. – A half-life of benzo(ghi)perylene in the presence of ozone was calculated to be approximately 1 minute. It requires 197 mg granular activated carbon per litre to reduce the concentration of benzo(ghi)perylene from 1.0 to 0.1 ppm at pH 7.0. (Sax 1986).
Total degradation in sediment	PAHs deposited in sediments are less subject to photochemical or biological oxidation, especially if the sediment is anoxic. Sedimentary PAH is therefore quite persistent and may accumulate to high concentrations (Sax 1986).
Other information about degradation	Airborne particulate PAHs can persist at relatively high concentrations in aerosols transported for long distances. The atmospheric persistence is longer than would be predicted from laboratory photo oxidation studies. On the other hand, The National Academy of Sciences (1972) proposed that the chemical half-life of PAH's in the atmosphere may be limited to hours or days (Sax 1986). Biodegradation is probably the ultimate fate process for benzo(ghi)perylene (Sax 1986). PAHs with 4 or more aromatic rings are degraded slowly by microbes. However, the concentrations of bacteria and fungi capable of oxidizing hydrocarbons are extremely low in all but heavily polluted fresh and marine waters. Most species cannot use PAHs as a sole carbon source. Microbial oxidation of PAHs requires oxygen an will not proceed in anoxic sediments or water (Sax 1986). During a 7 day incubation period with bacterial suspension of 1–2 ppm, an approximately 1% emulsion of benzo(ghi)perylene was degraded 60% (Sax 1986).

Metabolism in microorganisms	The soil bacterium Bacillus megaterium was found to metabolize benzo(ghi)perylene and certain other PAHs at the same rate regardless of concentrations or solubility in the medium (Sax 1986).
Other information about metabolism	There are large differences among aquatic species in their ability to absorb and assimilate PAH from food. Polychaete worms have a very limited ability; fish show limited and variable absorption from the gut; and crustaceans readily assimilate PAH. Assimilated PAHs are metabolized and excreted rapidly. For biomagnification to occur, a substance must be relatively resistant to metabolism or exretion (Sax 1986).
Bioconcentration factor, other organisms	68200 aquatic organisms containing 7.6% lipids (Sax 1986)
Other information about bioaccumulation	PAHs with 4 or more aromatic rings are metabolized slowly by multicellular organisms. Since the log octanol/water partition coefficient is high and metabolism is slow, benzo(ghi)perylene is probably bioaccumulated. In most cases PAHs are less bioavailable when complexed to colloidal organic materials or absorbed to organic or inorganic particulates than when in solution or in fine dispersion in water (Sax 1986).
Health effects	Not carcinogenic, but a cocarcinogen. PAHs presumably can be absorbed from ingestion, inhalation, and skin contact (Sax 1986).
Effects on wastewater treatment	Polychlorinated PAHs are probably highly toxic to aquatic organisms and persistent in the environment as are polychlorinated biphenyls and polychlorinated naphthalenes. Chlorination for purification of wastewaters or drinking waters containing high concentrations of PAHs may be inadvisable. Activated sludge treatment is unable to oxidize PAHs within normal retention times. – An overall reduction of benzo(ghi)perylene concentration of 88% from that in the intake river water (0.072 ppb) following water purification steps of holding in a reservoir, filtration, and chlorination was reported (Sax 1986).
Other information about water organisms	Lethal threshold concentration (LT50): Daphnia magna: 0.0002 mg/l, 0.58 days (Newsted & Giesy 1987).

252 • Benzo(k)fluoranthene 207-08-9

Synonyms	11,12-Benzofluoranthene B(k)F Dibenzo(b, jk)fluorene 8,9-Benzofluoranthene
Sumformula of the chemical	C20H12
State and appearance	Colourless needles.
Molecular weight	252.32
Melting point, °C	217
Log octanol/water coefficient, log Pow	6.84 (Sax 1986) 6.06 (Sax 1986)
Volatilization	Evaporation of lower-molecular-weight PAH's may be significant only in a clear, rapidly flowing shallow stream (Sax 1986).
Adsorption/desorption	Movement via sediment is an important transport process. An exchange equilibrium exists in natural water systems between absorbed and soluble PAHs. Although the particulate form is favored, a significant fraction of the PAH will be dissolved except in systems that are very heavily contaminated by PAHs. – It requires 18 mg granular activated carbon per litre to reduce the concentration of benzo(k)fluoranthene from 1.0 to 0.1 ppm at pH 7.1 (Sax 1986).
Photochemical degradation in air	The most common photo oxidation product in solution is an endo peroxide. Dealkylation, ring cleavage, and other reactions ensue following photo lysis or pyrolysis of these peroxides. Frequently, only quinones are isolable. Phodimers may result in some cases. Absorbed PAHs are more reactive than in solution (Sax 1986).

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Photochemical degradation in water	Photo lysis in an aquatic environment may be an important fate process, especially for the dissolved portion (Sax 1986).
Hydrolysis in water	Hydrolysis is not significant (Sax 1986).
Oxidation-reduction reactions	Ozone and chlorinating agents oxidize polycyclic aromatic hydrocarbons to quinones, diacids, and nuclear and side-chain oxidation products. Chlorinating agents also produce chlorine-substituted derivatives. - Oxidation of any PAH by chlorine and ozone, when used for the disinfection of drinking water, forms quinones. The half-life for the reaction of chlorine with all PAHs is less than 0.5 hr (Sax 1986).
Total degradation in sediment	PAHs deposited in sediments are less subject to photochemical or biological oxidation, especially if the sediment is anoxic. Sedimentary PAH is therefore quite persistent and may accumulate to high concentrations (Sax 1986).
Other information about degradation	Airborne particulate PAHs can persist at relatively high concentrations in aerosols transported for long distances. The atmospheric persistence is longer than would be predicted from laboratory photo oxidation studies. On the other hand, The National Academy of Sciences (1972) proposed that the chemical half-life of PAH's in the atmosphere may be limited to hours or days (Sax 1986). PAH's with fewer than 4 rings are degraded by microbes and are readily metabolized by multicellular organisms. – Biodegradation is probably the ultimate fate process for benzo(k)fluoranthene (Sax 1986). However, the concentrations of bacteria and fungi capable of oxidizing hydrocarbons are extremely low in all but heavily polluted fresh and marine waters. Most species cannot use PAHs as a sole carbon source. Microbial oxidation of PAHs requires oxygen and will not proceed in anoxic sediments or water (Sax 1986). During a 7 day incubation period with a bacterial suspension of 1–2 ppm, an approximately 1% emulsion of benzo(k)fluoranthene was degraded 54% (Sax 1986).
Other information about metabolism	There are large differences among aquatic species in their ability to absorb and assimilate PAH from food. Polychaete worms have a very limited ability; fish show limited and variable absorption from the gut; and crustaceans readily assimilate PAH. Assimilated PAHs are metabolized and excreted rapidly. For biomagnification to occur, a substance must be relatively resistant to metabolism or exretion (Sax 1986).
Bioconcentration factor, other organisms	28200 aquatic organisms containing 7.6% lipids (Sax 1986)
Other information about bioaccumulation	In most cases PAHs are less bioavailable when complexed to colloidal organic materials or adsorbed to organic or inorganic particulated than when in solution or in fine dispersion in water (Sax 1986).
TDLo values to mammals in non-oral exposure, mg/kg	2820 skn-mus, 47W-I, tumorigenic 72 scu-mus, 9W-I, tumorigenic (Sax 1986)
Health effects	Acute hazard level: PAH's can presumably be absorbed from ingestion, inhalation, and in skin contact (Sax 1986).
Carcinogenicity	Benzo(k)fluoranthene was rated not carcinogenic by the National Academy of Sciences (Sax 1986).
Mutagenicity	Mutagen data: mma, dat, 0.010 mg/plate (Sax 1986).
Effects on wastewater treatment	An 86% overall reduction of the b, j, and k isomers from their original total concentration in the river intake water of 0.147 ppb following the water purification steps of holding in a reservoir, filtration and chlorination was found. - Polychlorinated PAHs are probably highly toxic to aquatic organisms and persistent in the environment as are polychlorinated biphenyls and polychlorinated naphthalenes. Chlorination for purification of waste waters or drinking waters containing high concentrations of PAHs may be inadvisable. Activated sludge treatment is unable to oxidize PAHs within normal retention times (Sax 1986).

Other information about water organisms	Lethal threshold concentration (LT50): 0.0014 mg/l, 0.54 days, Daphnia magna (Newsted & Giesy 1987).

253 • Benzofuran

271-89-6

Synonyms	Coumarone
Sumformula of the chemical	C8H60
Log octanol/water coefficient, log Pow	2.67 (Sangster 1989)

254 • Benzoic acid

65-85-0

Sumformula of the chemical	C7H602
Use	Food preservative; pharmaceutical and cosmetic preparations; manufacturing of alkyl resins; intermediate in the synthesis of dyestuffs and pharmaceuticals; production of phenol and caprolactam; plasticizer manufacturing (to modify resins-PVC, PV acetate, phenol-formaldehyde).
State and appearance	White powder.
Molecular weight	122.1
Specific gravity (water=1)	1.27
Vapour density (air=1)	4.21
Water solubility, mg/l	2700 at 18 °C 3400 at 25 °C, 3000 (MITI 1992)
Melting point, °C	122 (MITI 1992)
Boiling point, °C	255 (MITI 1992)
pKa	4.2
Log octanol/water coefficient, log Pow	1.87 at 20 °C 1.9 (Anon. 1986) 1.87 (Hansch & Leo 1979) 2.03 (Lu & Metcalf 1975) 1.87 (Verschueren 1983) 1.87 (Sangster 1989)
Henry's law constant, Pa x m³/mol	0.0396 calc. (Suntio et al. 1988) 0.00415 calc. (Yaws et al. 1991)
Total degradation in water	Biodegradation: 85% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
Other information about degradation	Decomposition period by a soil microflora: 1 day (Verschueren 1983). Lag period for degradation of 16 mg/l by waste water or by soil at pH 7.3 and 30 °C: less than 1 day (Haller 1978).
LD50 values to mammals in oral exposure, mg/kg	1700 orl-rat (Patty 1967)
Carcinogenicity	Carcinogenicity: none (McCann et al. 1975).

Mutagenicity	Mutagenicity in the Salmonella test: none; < 0.0009 revertant colonies/nmol < 70 revertant colonies at 1 mg/plate (McCann et al. 1975).
LD50 values to birds in oral exposure, mg/kg	> 100 orl-Agelaius phoeniceus > 100 orl-Sturnus vulgaris (Schafer et al. 1983)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 480 mg/l (Bringmann & Kühn 1980).
LOEC values to algae, mg/l	55 rpd, schr, Microcystis aeruginosa (Bringmann & Kuhn 1976) 1630 rpd, schr, Scenedesmus quadricauda (Bringmann & Kuhn 1980a)
LC50 values to fishes, mg/l	180 96 hr, Gambusia affinis (Jones 1971)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): Algae (Microcystis aeruginosa): 55 mg/l (Bringmann & Kühn 1976) Green algae (Scenedesmus quadricauda): 1630 mg/l Protozoa (Entosiphon sulcatum: 218 mg/l Protozoa (Uronema parduczi): 31 mg/l (Bringmann & Kühn 1980a) Arthropoda: Daphnia magna: immobilization at 146 mg/l; prolonged exposure (McKee & Wolf 1963).
Other information	Natural sources (water and air): cranberries, prunes, ripe cloves, bark of wild black cherry tree, scent glands of beavers, and oil of anise seeds (Verschueren 1983).

255 • Benzoine 119-53-9

Synonyms	Benzoin	
Water solubility, mg/l	28	(MITI 1992)
Melting point, °C	134	(MITI 1992)
Boiling point, °C	344	(MITI 1992)
Total degradation in water	Biodegradation: 85% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LD50 values to birds in oral exposure, mg/kg	> 98.0	orl-Agelaius phoeniceus (Schafer et al. 1983)

256 • Benzonitrile 100-47-0

Synonyms	Benzenecarbonitrile Phenylcyanide	
Sumformula of the chemical	C7H5N	
Molecular weight	103.12	
Specific gravity (water=1)	1.01	at 15/15 °C
Water solubility, mg/l	10000 10000	at 100 °C (MITI 1992)

Melting point, °C	-14.3 (MITI 1992)
Boiling point, °C	190.7 (MITI 1992)
Log octanol/water coefficient, log Pow	1.55 (Anon. 1986) 1.56 (Sangster 1989)
Henry's law constant, Pa x m³/mol	55.33 calc. (Yaws et al. 1991)
Total degradation in water	Biodegradation: 63.4% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
LD50 values to birds in oral exposure, mg/kg	> 100 orl-Agelaius phoeniceus > 100 orl-Sturnus vulgaris (Schafer et al. 1983)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): Bacteria (Pseudomonas putida): 11 mg/l (Bringmann & Kühn 1980).
LOEC values to algae, mg/l	3.4 rpd, schr, Microcystis aeruginosa (Bringmann & Kuhn 1976) 75 rpd, schr, Scenedesmus quadricauda (Bringmann & Kuhn 1980a)
LC50 values to fishes, mg/l	78 96 hr, Pimephales promelas 400 96 hr, Lepomis macrochirus (Jones 1971) 78 96 hr, Lepomis macrochirus (Henderson et al. 1960) 130 96 hr, Branchydanio rerio 54–97 48 hr, Leuciscus idus (Wellens 1982)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): Algae (Microcystis aeruginosa): 3.4 mg/l (Bringmann & Kühn 1976) Green algae (Scenedesmus quadricauda): 75 mg/l Protozoa (Entosiphon sulcatum): 30 mg/l Protozoa (Uronema parduczi): 119 mg/l (Bringmann & Kühn 1980). Adult bluegills: no organoleptic influence at 35 mg/l (McKee & Wolf 1963).

257 • Benzophenone

119-61-9

Sumformula of the chemical	C13H10O
Water solubility, mg/l	45 (MITI 1992)
Melting point, °C	49 (MITI 1992)
Boiling point, °C	306 (MITI 1992)
Log octanol/water coefficient, log Pow	3.18 (Anon. 1986) 3.18 (Sangster 1989)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

Bioconcentration factor, fishes	3.4–9.2 6w, Cyprinus carpio, conc 0.3 mg/l 3.4–12 6w, Cyprinus carpio, conc 0.3 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	15.3 96 hr, Pimephales promelas (Veith et al. 1983) 27 48hr, Oryzias latipes (MITI 1992)

258 • 1,4-Benzoquinone 106-51-4

Synonyms	p-Benzoquinone 2,5-Cyclohexadien-1,4-dione 1,4-Benzoquinone Quinone
Use	Manufacture of dyes and hydroquinone.
State and appearance	Yellow crystals.
Odour	Characteristic, pungent. Absolute perception limit: 0.1 ppm 100% recognition: 0.15 ppm Odour index at 20 °C: 790 (Verschueren 1983)
Molecular weight	108.09
Specific gravity (water=1)	1.318 at 20 °C
Conversion factor, 1 ppm in air=	4.49 mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.226 ppm
Vapour pressure, mmHg	0.09 at 20 °C
Degradation point, °C	115–124
Log octanol/water coefficient, log Pow	0.2
Other information about degradation	Impact on biodegradation processes: at 0.2 mg/l inhibition of degradation of glucose by Pseudomonas fluorescens; at 55 mg/l inhibition of degradation of glucose by Escherichia coli (Bringmann & Kühn 1960).
LD50 values to mammals in oral exposure, mg/kg	130–296 orl-rat (Verschueren 1983)
LD50 values to mammals in non-oral exposure, mg/kg	25 par-rat 94 par-mus (Verschueren 1983)
LC50 values to mammals in inhalation exposure, mg/m^3	250 ihl-mus, 2 hr (Verschueren 1983)
Other information about mammals	Rat: inhalation LC100: 230–270 mg/m^3, 2 hr Mouse: inhalation: LC100: 320–340 mg/m^3, 2 hr (Verschueren 1983).
Health effects	Man: eye irritation from 0.1 ppm (Verschueren 1983).
Effects on microorganisms	Bacteria: Escherichia coli: toxic: 55 mg/l (Meinck et al. 1970).

EC50 values to microorganism, mg/l	12 OECD 209 (King and Painter 1985) 10 Nitrification (King and Painter 1985) 2.4 16 hr Growth (King and Painter 1985)
LC50 values to fishes, mg/l	0.125 96 hr, Salmo gairdneri 0.045 96 hr, Pimephales promelas (DeGraeve et al. 1980)
Effects on the physiology of water organisms	Inhibition of photosynthesis of a fresh water non-axenic uni-algal culture of Selenastrum capricornutum: at 0.1 mg/l: 37% carbon-14 fixation (vs.controls) at 1 mg/l: 17% carbon-14 fixation (vs.controls) at 10 mg/l: 7–13% carbon-14 fixation (vs.controls) at 100 mg/l: 1% carbon-14 fixation (vs.controls) at 1000 mg/l: 2% carbon-14 fixation (vs.controls) (Verschueren 1983).
Other information about water organisms	Algae: blue algae: toxic: < 1 mg/l Scenedesmus: toxic: 6 mg/l (Meinck et al. 1970). Arthropoda: Daphnia: toxic: 0.4 mg/l (Verschueren 1983). Fish: Pimephales promelas: probable toxic conc.: < 0.1 mg/l after 120 hr (Verschueren 1983).
Other effects on aquatic ecosystems	Reduction of amenities: taste: average: 0.71 mg/l range 0.016–4.3 mg/l (Meinck et al. 1970). Tainting of fish flesh: 0.5 mg/l (Verschueren 1983).

259 • Benzothiazole

95-16-9

Sumformula of the chemical	C7H5NS
EINECS-number	2023962
Water solubility, mg/l	4300 (MITI 1992)
Melting point, °C	< -10 (MITI 1992)
Boiling point, °C	223–225 (MITI 1992)
Log octanol/water coefficient, log Pow	2.01 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	2.1–5.1 6w, Cyprinus carpio, conc 0.2 mg/l < 4.1–7.5 6w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
LC50 values to fishes, mg/l	87.2 48hr, Oryzias latipes (MITI 1992)

260 • Benzotrichloride 98-07-7

Synonyms	Phenylchloroform Toluenetrichloride Benzenyltrichloride Benzoic trichloride Benzyltrichloride Trichloromethyl benzene
State and appearance	Colourless to yellowish liquid.
Odour	Penetrating odour.
Specific gravity (water=1)	1.38
Melting point, °C	-5
Boiling point, °C	213–214
LD50 values to birds in oral exposure, mg/kg	> 100 orl-Agelaius phoeniceus (Schafer et al. 1983)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): Bacteria (Pseudomonas putida): > 100 mg/l (Bringmann & Kühn 1980).
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): Green algae (Scenedesmus quadricauda): > 100 mg/l Protozoa (Entosiphon sulcatum): 56 mg/l Protozoa (Uronema parduczi: > 80 mg/l (Bringmann & Kühn 1980).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

261 • Benzotrifluoride 98-08-8

Synonyms	Toluene trifluoride Trifluoromethylbenzene
Sumformula of the chemical	$C_6H_5F_3$
Use	Intermediate for dyes, and pharmaceuticals; solvent and dielectric fluid; vulcanizing agent; insecticides.
State and appearance	Water-white liquid.
Odour	Aromatic odour.
Water solubility, mg/l	140 (MITI 1992)
Boiling point, °C	102.1 98–99/725 mmHg (MITI 1992)
Flashing point, °C	12.2
Log octanol/water coefficient, log Pow	3.31 (MITI 1992)
Other physicochemical properties	Miscible with alcohol, acetone, benzene, carbon tetrachloride, ether, n-heptane; insoluble in water. Flammable, dangerous fire risk (Sax & Lewis 1987).

Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 2.4 mg/l sludge: 2 mg/l 0% by BOD period: 28d substance: 11.9 mg/l sludge: 2 mg/l (MITI 1992).	
Bioconcentration factor, fishes	26–54 31–58	6w, Cyprinus carpio, conc 0.1 mg/l 6w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).v	
Health effects	Highly toxic by inhalation (Sax & Lewis 1987).	
LC50 values to fishes, mg/l	28	48hr, Oryzias latipes (MITI 1992)

262 • Benzoyl chloride 98-88-4

Synonyms	Benzenecarbonylchloride	
Molecular weight	140.57	
Specific gravity (water=1)	1.22	at 15/15°C
Vapour density (air=1)	4.88	
Conversion factor, 1 ppm in air=	5.84	mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.17	ppm
Vapour pressure, mmHg	0.4 1	at 20°C at 32°C
Melting point, °C	-1	
Boiling point, °C	197	
LC50 values to crustaceans, mg/l	180	96 hr, Palaemonetes pugio (Curtis et al. 1979)
LC50 values to fishes, mg/l	35	96 hr, Pimephales promelas (Curtis et al. 1979)

263 • Benzoylamino acetic acid 495-69-2

Synonyms	Hippuric acid Benzaminoacetic acid Benzoylglycine	
Water solubility, mg/l	4000	MITI 1992
Melting point,°C	187–188	MITI 1992
Total degradation in water	Biodegradation: 81% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

Ready biodegradability	Confirmed to be biodegradable (Anon. 1987)
LD50 values to birds in oral exposure, mg/kg	> 101 orl-Agelaius phoeniceus (Schafer et al. 1983)

B

264 • Benzoylprop ethyl 22212-55-1

Use	Herbicide.
LC50 values to fishes, mg/l	2.2 96 hr, Salmo gairdneri (Pesticide Manual 1983)

265 • Benzthiazuron 1929-88-0

Synonyms	N-(2-Benzothiazolyl)-N'-methylurea
State and appearance	White powder.
Vapour pressure, mmHg	0.00001 at 90 °C
Degradation point, °C	287
LD50 values to mammals in oral exposure, mg/kg	1280 orl-rat (Martin 1968)
Other information about mammals	Dermal applications of 500 mg/kg gave no symptoms; in diet: all rats tested in 60 days feeding tests at 130 mg/kg survived (Martin 1968).
LC50 values to fishes, mg/l	400 96 hr, Rasbora heteromorpha (Tooby et al. 1975)

266 • N-Benzyl acetamide 588-46-5

Melting point, °C	63 (MITI 1992)
Total degradation in water	Biodegradation: 77% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

267 • Benzyl acetate 140-11-4

Synonyms	Acetic acid, phenylmethyl ester
Sumformula of the chemical	C9H1002
EINECS-number	2053997
Water solubility, mg/l	3100 (MITI 1992)
Melting point, °C	-51 (MITI 1992)
Boiling point, °C	216 (MITI 1992)
Total degradation in water	Biodegradataion: 92–96% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

268 • Benzyl amine

100-46-9

Synonyms	α-Aminotoluene
Sumformula of the chemical	C7H9N
Use	Chemical intermediate for dyes, pharmaceuticals, polymers.
Molecular weight	107.15
Specific gravity (water=1)	0.983 at 19/4 °C
Water solubility, mg/l	> 100 (MITI 1992)
Boiling point, °C	185 (MITI 1992)
Log octanol/water coefficient, log Pow	1.09 (Sangster 1989)
Total degradation in water	Biodegradation: 52–75% (NO2) by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l 62–91% (NH3) by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
Other information about degradation	Impact on biodegradation processes: inhibition of degradation of glucose by Pseudomonas fluorescens at: 400 mg/l; inhibition of degradation of glucose by Escherichia coli at: > 1000 mg/l (Bringmann & Kühn 1960). NH3 oxidation by Nitrosomonas sp.: at 100 mg/l: 26% inhibition at 50 mg/l: 10% inhibition at 10 mg/l: 0% inhibition (Hockenbury & Grady 1977).
Effects on microorganisms	Bacteria: Escherichia coli: no effect at 1 g/l (Meinck et al. 1970).
Other information about water organisms	Algae: Scenedesmus: toxic: 6 mg/l Arthropoda: Daphnia: toxic: 60 mg/l (Meinck et al. 1970).

269 • Benzyl benzoate

120-51-4

Synonyms	Benzoic acid, benzyl ester
Sumformula of the chemical	C14H12O2
Use	Fixative and solvent for musk in perfumes and flavors; medicine (external); plasticizer for nitrcellulose and celluiose acetate; miticide.
State and appearance	Water-white liquid; readly freezes.
Odour	Sharp, burning taste and faint aromatic odour.
Specific gravity (water=1)	1.116–1.120 (25/25 °C)
Melting point, °C	18.8
Boiling point, °C	325
Flashing point, °C	147.7

Log octanol/water coefficient, log Pow	3.97 3.97	(Anon. 1986) (Sangster 1989)
Other physicochemical properties	Supercools easily. Insoluble in water, glycerol; soluble in alcohol, chloroform, ether. Combustible.	

B

270 • Benzyl chloride 100-44-7

Synonyms	α-Chlorotoluene	
Sumformula of the chemical	C7H7Cl	
Use	Dyes, intermediate.	
Odour	Characteristic. Lacrimator aromatic. Threshold values: 0.25 mg/m³ = 0.047 ppm; 0.04 ppm (Hovious et al. 1973 (Verschueren 1983). PIT50% (Population Identification Threshold): 0.01 ppm PIT100%: 0.047 ppm (Verschueren 1983).	
Molecular weight	126.59	
Specific gravity (water=1)	1.102	at 18/4 °C
Vapour density (air=1)	4.36	
Conversion factor, 1 ppm in air=	5.262	mg/m³
Conversion factor, 1 mg/m³ in air=	0.19	ppm
Vapour pressure, mmHg	1 1.7 3.62	22 °C 30 °C mmHg/37.8 °C (MITI 1992)
Melting point, °C	-41/-43	
Boiling point, °C	179.4	(MITI 1992)
Log octanol/water coefficient, log Pow	2.3	(Sangster 1989)
Total degradation in water	Biodegradation: 71% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	1231	orl-rat (Lewis & Sweet 1984)
LC50 values to mammals in inhalation exposure, ppm	150	2 hr, ihl-rat (Lewis & Sweet 1984)
Mutagenicity	Mutagenicity in the Salmonella test: weakly mutagenic (without liver homogenate): 0.02 revertant colonies/nmol; 230 revertant colonies at 2 mg/plate (McCann et al. 1975).	
Effects on microorganisms	Bacteria: Pseudomonas putida: inhibition of cell multiplication starts at 4.8 mg/l (Bringmann & Kühn 1976).	

LOEC values to algae, mg/l	30	rpd, schr, Microcystis aeruginosa (Bringmann & Kuhn 1976)
LC50 values to crustaceans, mg/l	3.9	96 hr, Penaeus setiferus (Curtis et al. 1979)
LC50 values to fishes, mg/l	4 3–16 0.4 6	96hr, Branchydanio rerio 48 hr, Leuciscus idus (Wellens 1982) 14 d, Poecilia reticulata (Hermens et al. 1985) 96 hr, Pimephales promelas (Curtis et al. 1979)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): algae (Microcystis aeruginosa): 30 mg/l (Bringmann & Kühn 1976) green algae (Scenedesmus quadricauda): 50 mg/l protozoa (Entosiphon sulcatum): 25 mg/l protozoa (Uronema parduczi): 50 mg/l (Bringmann & Kühn 1980). Protozoa: Vorticela campanula: toxic: 11 mg/l Paramaecium caudatum: toxic: 800 mg/l Fish: Trutta iridea: paralysis: 10 mg/l Cyprinus carpio: paralysis: 17 mg/l (Meinck et al. 1970).	
Other effects on aquatic ecosystems	Reduction of amenities: faint odour: 0.0016 mg/l (Verschueren 1983).	

271 • Benzyl pyridyne

2116-65-6

LD50 values to birds in oral exposure, mg/kg	> 17.8 > 100	orl-Agelaius phoeniceus orl-Sturnus vulgaris (Schafer et al. 1983)
Other information about water organisms	EC50, 60hr, 36 mg/l, rpd, Tetrahymena pyriformis (Schultz & Moulton 1985).	

272 • Benzyl trimethyl ammonium chloride

56-93-9

Synonyms	Trimethylbenzylammonium chloryde	
Total degradation in water	Biodegradation: 1% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.2 < 1.5	6w, Cyprinus carpio, conc 2 mg/l 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	> 1000	48hr, Oryzias latipes (MITI 1992)

273 • 4-Benzylphenol

101-53-1

Synonyms	4-Hydroxy diphenylmethane	
Water solubility, mg/l	73.2	(MITI 1992)

Melting point, °C	84	(MITI 1992)
Boiling point, °C	320–322	(MITI 1992)
Log octanol/water coefficient, log Pow	3.47	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	18–38 10–32	6w, Cyprinus carpio, conc 0.03 mg/l 6w, Cyprinus carpio, conc 0.003 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	3.05	48 hr, Oryzias latipes (MITI 1992)

274 • Beryllium and beryllium compounds 7440-41-7

LC50 values to crustaceans, mg/l	1	48 hr, Daphnia magna (LeBlanc 1980)
LC50 values to fishes, mg/l	0.38	28 d, Salmo gairdneri (Birge et al. 1980)

275 • Bibenzyl 103-29-7

Synonyms	Dibenzyl 1,2-Diphenylethane	
Sumformula of the chemical	C14H14	
Use	Organic synthesis.	
Molecular weight	182.27	
Specific gravity (water=1)	1.014	
Melting point, °C	50–53	
Boiling point, °C	284	
Log octanol/water coefficient, log Pow	4.7	(Sangster 1989)

276 • Bicyclo(2.2.1)hepta-2,5-diene 121-46-0

Sumformula of the chemical	C7H8	
Chemical oxygen demand, g 02/g	2.36	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.23	5 days (Bridie et al.1979)

277 • Bifenox

42576-02-3

Synonyms	Methyl 5-(2,4-dichlorophenoxy)-2-nitrobenzoate
Effects on plants	1.0 kg bifenox/ha was applied with a sprayer following seeding (preemergence) to lamb's-quarters (Chenopodium album L.) → plants (seeds) were killed (Jensen et al. 1977).

278 • Binapacryl

485-31-4

Synonyms	2-(1-Methyl-n-propyl)-4,6-dinitrophenyl-2-methylcrotonate 2-sec-Butyl-4,6-dinitrophenyl-3-methyl-2-butenoate 2(2-Butyl-4,6-dinitrophenyl)-3,3-dimethylacrylate
Use	Fungicide; acaricide; contact miticide.
State and appearance	Crystalline solid.
Specific gravity (water=1)	1.156
Melting point, °C	65–69
LD50 values to mammals in oral exposure, mg/kg	120–165 orl-rat 1600 orl-mus 300 orl-gpg (Verschueren 1983)
LD50 values to mammals in non-oral exposure, mg/kg	750 in acetone, skn-rbt (Verschueren 1983)
Effects on the physiology of mammals	Dogs: 50 mg/kg causes vomiting and hypernoea; Mice: acute dermal LD50: no death up to 1000 mg/kg as an acacia suspension (Verschueren 1983). Chronic toxicity: rats: 200 ppm for 2 years without reaction 500 ppm for 2 years, only small reduction in body weight dogs: 40 ppm over 2 years without reaction (Verschueren 1983).
Other information about birds	Chickens: single oral doses tolereted up to 800 mg/kg (Verschueren 1983).
LOEC values to fishes, mg/l	0.06 act, Salmo salar (Zitko et al.1976)
Other information about water organisms	Fish: guppies: LD100: 1 ppm (Verschueren 1983).

279 • Bioresmethrin *

28434-01-7

Synonyms	NRDC 107
Active ingredients	Fennosan F50; Slimacide V10
Use	Insecticide.
LC50 values to fishes, mg/l	0.014 96hr, Rasbora heteromorpha (Tooby et al. 1975)

280 • Biphenyl

92-52-4

Synonyms	Diphenyl
Sumformula of the chemical	$C_{12}H_{10}$
Use	Fungicide, organic synthesis, heat-transfer agent, plant disease control, manufacture of benzidine, dyeing assistant for polyesters.

State and appearance	White scales.	
Odour	Pleasant odour.	
Molecular weight	154.22	
Specific gravity (water=1)	1	approximately
Water solubility, mg/l	7.5	
Melting point, °C	70	(MITI 1992)
Boiling point, °C	255.2	(MITI 1992)
Flashing point, °C	112.7	
Log octanol/water coefficient, log Pow	3.95 3.95 3.88 4.09 3.98	(Anon. 1986) (Chin et al. 1986) (Mackay 1982) (Hawker & Connell 1985) (Sangster 1989)
Henry's law constant, Pa x m³/mol	86.53	calc. ((Yaws et al. 1991))
Other physico–chemical properties	Soluble in alcohol and ether, insoluble in water.	
Half-life in water, days	0.31	calculated, 25 °C, 1 m depht (Verschueren 1983)
Total degradation in water	Biodegradation: 66% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
Bioconcentration factor, fishes	437	Salmo gairdneri (Verschueren 1983)
Bioconcentration factor, other organisms	307	in whole cells (Marine yeast) (Verschueren 1983)
LD50 values to mammals in oral exposure, mg/kg	3280 2400	orl-rat orl-rbt (Lewis & Sweet 1984)
TCLo values to mammals in inhalation exposure, mg/kg	4.4	ihl-hmn (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	> 96	orl- Agelaius phoeniceus (Schafer et al. 1983)
LC50 values to crustaceans, mg/l	4.7	48 hr, Daphnia magna (LeBlanc 1980)

281 • 2-Biphenyl amine 90-41-5

Synonyms	2-Aminobiphenyl o-Aminobiphenyl	
Sumformula of the chemical	C12H11N	
Water solubility, mg/l	410	(MITI 1992)
Melting point, °C	49–50	(MITI 1992)
Boiling point, °C	299	(MITI 1992)

pKa	3.82	at 22 °C (Sangster)
Log octanol/water coefficient, log Pow	2.84 2.72	(Sangster 1989) (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	10–31 10–42	6w, Cyprinus carpio, conc 0.2 mg/l 6w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	22.8	48 hr, Oryzias latipes (MITI 1992)

282 • 2,2'-Biphenyl dicarboxylic acid 482-05-3

Water solubility, mg/l	100	(MITI 1992)
Melting point, °C	228–229	(MITI 1992)
Total degradation in water	Biodegradation: 81–136% by BOD period: 21d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	

283 • 2,2'-Bipyridine 366-18-7

Synonyms	2,2'-Dipyridyl
Use	Iron-chelating agent.
Molecular weight	156.19
Melting point, °C	70–73
Boiling point, °C	273
Other information about degradation	Impact on biodegradation processes: NH_3 oxidation by Nitrosomonas: at 100 mg/l: 91% inhibition at 50 mg/l: 81% inhibition at 10 mg/l: 23% inhibition (Hockenbury & Grady 1977).

284 • Bis(2-(2-butoxy ethoxy)ethyl) adipate 141-17-3

Synonyms	Di(butoxyethoxyethyl)adipate	
Melting point, °C	-47	(MITI 1992)
Boiling point, °C	240	5 mmHg (MITI 1992)

Total degradation in water	Biodegradation: 86% by BOD period: 14d substance: 100mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

285 • Bis(2,3,5-trichloro-6-hydroxyphenyl)methane 70-30-4

Sumformula of the chemical	C13H6C1602	
EINECS-number	2007338	
Water solubility, mg/l	> 10	(MITI 1992)
Melting point, °C	164–165	(MITI 1992)
Log octanol/water coefficient, log Pow	5.94	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	87–148 82–153	8w, Cyprinus carpio, conc 0.002 mg/l 8w, Cyprinus carpio, conc 0.0002 mg/l (MITI 1992)
LC50 values to fishes, mg/l	0.338	48hr, Oryzias latipes (MITI 1992)

286 • N,N-Bis(2,3-epoxypropyl)aniline 2095-06-9

Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).

287 • Bis(2,4-dichlorobenzoyl) peroxide 133-14-2

Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

288 • N,N'-Bis(2-aminoethyl)ethylene diamine 112-24-3

Synonyms	Tetraethylenetetramine	
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LD50 values to birds in oral exposure, mg/kg	> 101	orl-Agelaius phoeniceus (Schafer et al. 1983)

289 • Bis(2-chloroethyl)ether 111-44-4

Synonyms	Dichloroether Dichlorodiethyl ether 2,2'-Dichlorodiethyl ether Bis(β-chloroethyl) ether Chlorex 1-Chloro-2-(β-chloroethoxy)ethane Chloroethylether Clorex 2,2'-Dichloroethyl ether β, β-Dichlorodiethyl ether Dichloroethyl ether Di(2-chloroethyl) ether Dichloroethyl oxide 1,1'-Oxybis(2-chloro)ethane	
Sumformula of the chemical	C4H8Cl2O	
Use	Solvent.	
Molecular weight	143.02	
Water solubility, mg/l	10200	20 °C
Melting point, °C	-46	(MITI 1992)
Boiling point, °C	179.2	(MITI 1992)
Total degradation in water	Biodegradation: 8.3% by BOD period: 21dv substance: 100 mg/l sludge 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).	
Bioconcentration factor, fishes	0.4–1.3 < 10	6w, Cyprinus carpio, conc 3 mg/l 6w, Cyprinus carpio, conc 0.3 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	75 112	orl-rat orl-mus (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	300 720	skn-gpg skn-rbt (Sweet 1987)
LC50 values to mammals in inhalation exposure, mg/m³	650 330	ihl-mus, 2hr ihl-rat, 4hr (Sweet 1987)
TDLo values to mammals in oral exposure, mg/kg	33	orl-mus, tumorigenic (Sweet 1987)
TDLo values to mammals in non-oral exposure, mg/kg	2400	scu-mus, tumorigenic (Sweet 1987)
LC50 values to crustaceans, mg/l	240	48 hr, Daphnia magna, LeBlanc 1980
LC50 values to fishes, mg/l	600 610	96 hr, Lepomis macrochirus (Buccafusco et al. 1981) 48hr, Oryzias latipes (MITI 1992)

B

290 • 2,2-Bis(3,5-Dibromo-4-(2-hydroxy ethoxy) phenyl)propane 4162-45-2

Bioconcentration factor, fishes	10.0–35.5 Cyprinus carpio, conc 0.25 mg/l 14.8–53.0 Cyprinus carpio, conc 0.025 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	30 48 hr, Oryzias latipes (MITI 1992)

291 • 2,2-Bis(4-hydroxy-3,5-dibromophenyl) propane 79-94-7

Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Bioconcentration factor, fishes	30–341 8w, Cyprinus carpio, conc 0.08 mg/l 52–485 8w, Cyprinus carpio, conc 0.008 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon.1987).
LC50 values to fishes, mg/l	8.2 48 hr, Oryzias latipes (MITI 1992)

292 • 2,2-Bis(4-hydroxyphenyl) propane 80-05-7

Melting point, °C	155–156 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substace: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Bioconcentration factor, fishes	5.1–13.3 6w, Cyprinus carpio, conc 0.150 mg/l < 20–67.7 6w, Cyprinus carpio, conc 0.015 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	15 48 hr, Oryzias latipes (MITI 1992)

293 • Bis(aminoethyl) amine 111-40-0

Melting point, °C	-39	(MITI 1992)
Boiling point, °C	208	(MITI 1992)

Log octanol/water coefficient, log Pow	< -3 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factorfishes	< 0.3–1.7 6w, Cyprinus carpio, conc 2 mg/l < 2.8–6.3 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	780 48hr, Oryzias latipes (MITI 1992)

294 • 1,3-Bis(aminomethyl) benzene 1477-55-0

Melting point, °C	13 (MITI 1992)
Boiling point, °C	245–248 (MITI 1992)
Total degradation in water	Biodegradation: 22% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.3 6w, Cyprinus carpio, conc 2 mg/l < 2.7 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	155.88 48 hr, Oryzias latipes (MITI 1992)

295 • 1,4-Bis(benzoyloxyimino)-2,5-cyclohexadiene 120-52-5

Synonyms	p, p'-Dibenzoylquinonedioxime
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.54–1.2 6w, Cyprinus carpio, conc 0.07 mg/l < 4.9–8.0 6w, Cyprinus carpio, conc 0.007 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	> 50 48 hr, Oryzis latipes (MITI 1992)

296 • Bis(chloromethyl)naphthalene 27156-22-5

Sumformula of the chemical	C12H10Cl2	
Molecular weight	225.12	
Vapour density (air=1)	7.78	
Conversion factor, 1 ppm in air=	9.36	mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.11	ppm
Half-life in water, days	0.031	45.2 min., evaporation, from 1 ppm aqueous solution at 25 °C, still air and an average depth of 6.5 cm (Verschueren 1983)

297 • Bis(cyanoethyl)amine 111-94-4

Sumformula of the chemical	C6H9N3	
EINECS-number	2039223	
Water solubility	< 100000 (MITI 1992)	
Boiling point, °C	140–145 (MITI 1992)	
Log octanol/water coefficient, log Pow	–1.34	(MITI 1992)
Total degradation in water	Biodegradation: 1–3% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	0.2–0.4, 6w, Cyprinus carpio, conc. 1 mg/l < 1.2, 6w, Cyprinus carpio, conc. 0.1 mg/l (MITI 1992).	
LC50 values to fishes, mg/l	> 1000	48hr, Oryzias latipes (MITI 1992)

298 • 4,4'-Bis(dimethylamino)benzophenone 90-94-8

Synonyms	Michlers ketone	
Water solubility, mg/l	0.65	(MITI 1992)
Melting point, °C	179	(MITI 1992)
Log octanol/water coefficient, log Pow	4.05	(MITI 1992)
Bioconcentration factor, fishes	25–54 17–39	8W, Cyprinus carpio, conc 0.2 mg/l 8w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LD50 values to birds in oral exposure, mg/kg	100 > 316	orl-Agelaius phoeniceus orl-Coturnix coturnix (Schafer et al. 1983)
LC50 values to fishes, mg/l	> 250	48 hr, Oryzias latipes (MITI 1992)

299 • Bis(α,α-dimethylbenzyl)peroxide 80-43-3

Synonyms	Dicumyl peroxide	
Water solubility, mg/l	0.4	(MITI 1992)
Melting point, °C	40.6	(MITI 1992)
Log octanol/water coefficient, log Pow	5.5	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	137–1470 181–667	8w, Cyprinus carpio, conc 0.01 mg/l 8w, Cyprinus carpio, conc 0.001 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	4.2	48hr, Oryzias latipes (MITI 1992)

300 • 2',2'-Bis(methacryloyloxymethyl) butyl methacrylate 3290-92-4

Sumformula of the chemical	C18H26O6	
Water solubility, mg/l	13	(MITI 1992)
Melting point, °C	< -10	(MITI 1992)
Log octanol/water coefficient, log Pow	4.39	(MITI 1992)
Total degradation in water	Biodegradation: 50–59% by BOD (Tributylol propane was remained) period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

301 • Bis(N-cyclohexyl diazenium dioxy)-copper 15627-09-5

Synonyms	Copper-HDO Xyligen Cu Copper, bis(N-hydroxy-N-nitrosocyclohexanaminato-O, O')-
Sumformula of the chemical	C12H22CuN4O4
EINECS-number	2397034
Purity, %	> 98 (WPSREG 1993)
Known impurities	basic copper compounds 0.3% (WPSREG 1993).
Use	Active ingredient in liquid wood preservatives with preventive efficacy against wood-destroying fungi including softrot and wood-destroying insects (WPSREG 1993).

State and appearance	Crystalline powder (WPSREG 1993).
Molecular weight	349.88
Density, kg/m³	0.00028 (WPSREG 1993)
Vapour pressure, mmHg	< 0.00001, 20 °C, WPSREG 1993 < 0.00015, 80 °C (WPSREG 1993)
Water solubility, mg/l	35 pH 4.0, 23 °C 6.1 pH 7.0 8.6 pH 9.0 (WPSREG 1993)
Fat solubility, g/100g	0.49 37 °C (WPSREG. 1993)
Melting point, °C	157 (WPSREG. 1993)
Log octanol/water coefficient, log Pow	2.40–2.51 (WPSREG 1993)
Log soil organic carbon coefficient, log Koc	2.38–3.76 (HDO-compounds) (WPSREG 1993)
Adsorption/desorption	Desorption 7.6–86% of HDO adsorbed to soil (WPSREG 1993)
Other physicochemical properties	Solubility in organic solvents mg/100 ml (at room temperature): benzene 6 672 methylene chloride 16 430 ethylacetate 3 060 methanol 1 621 petroleum 77 trichloroethylene 9 070 o-xylene 2 904 chloroform 35 571 dioxane 4 235 isopropanol 396 ethylene glycol 233 dimethylformamide 10 333 toluene 3 724 dimethyl sulfoxide 13 224 (WPSREG 1993). Not inflammable (WPSREG 1993).
Hydrolysis in water	Stabile at pH 7 and 9 (50 °C) (WPSREG 1993).
Hydrolysis in acid	T1/2 = 3.0 d at pH 4 (50 °C), T1/2 = 3.9 d at pH 4 (35 °C) (WPSREG 1993).
LD50 values to mammals in oral exposure, mg/kg	740–1000 orl-mam (WPSREG 1993)
Other information about mammals	NOEL (3 mo) 35–41 mg/kg of body weight, orl-rat (WPSREG 1993).
Effects on invertebrates	LC50 636 mg/kg (14d) Eisenia foetida (WPSREG 1993).
EC50 values to algae, mg/l	0.056–0.095 EbC50 (72hr) Scenedesmus subspicatus 0.12–0.15 ErC50 (72hr) Scenedesmus subspicatus (WPSREG 1993)
NOEC values to algae, mg/l	0.056 72hr, Scenedesmus subspicatus (WPSREG 1993)
NOEC values to crustaceans, mg/l	0.75 48hr, Daphnia magna 0.75 21d, Daphnia magna (WPSREG 1993)

LC50 values to fishes, mg/l	0.22 0.46	0.22–0.46, 96hr, orl-Oncorhyncus mykiss (nominal consentrations, measured consentrations obviously under 80% of these) (WPSREG 1993)
Other information about water organisms	EC100 (48hr) 1.5, Daphnia magna EC100 (21d) 1.5, Daphnia magna (WPSREG. 1993)	

302 • N,N-Bis(octylphenyl) amine 26603-23-6

Melting point, °C	96.5	96.5–101 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 1 < 10	6w, Cyprinus carpio, conc 0.5 mg/l 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	> 1000	48hr, Oryzias latipes (MITI 1992)

303 • Bis(phenoxyarsinyl)oxide 58-36-6

Synonyms	DID 47	
Other information about mammals	ALD = 42.0 mg/kg, act, orl, deer mouse LDfr = 50.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).	
LD50 values to birds in oral exposure, mg/kg	23.7 100	orl-Agelaius phoeniceus orl-Passer domesticus (Schafer et al. 1983)

304 • 1,2-Bis(stearoylamino)ethane 110-30-5

Sumformula of the chemical	C38H76N2O2	
EINECS-number	2037556	
Water solubility, mg/l	< 4900	(MITI 1992)
Melting point, °C	142 ± 2	(MITI 1992)
Total degradation in water	Biodegradation: 1.1% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.7 < 6.2	6w, Cyprinus carpio, conc 0.830 mg/l, 6w, Cyprinus carpio, conc 0.083 mg/l, (MITI 1992)
LC50 values to fishes, mg/l	> 300	48 hr, Oryzias latipes (MITI 1992)

B

305 • 1,1-Bis(tert-butyldioxy)-3,3,5-trimethyl cyclohexane 6731-36-8

Water solubility, mg/l	0.6	(MITI 1992)
Melting point, °C	-30	(MITI 1992)
Log octanol/water coefficient, log Pow	6.53	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	3500–9860 4960–13200	8w, Cyprinus carpio, conc 0.2 mg/l 8w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 500	48 hr, Oryzias latipes (MITI 1992)

306 • Bis(tri-n-butyltin)dibromosuccinate 31732-71-5

Water solubility, mg/l	< 5	(MITI 1992)
Melting point, °C	145.2–146.6	(MITI 1992)
Total degradation in water	Biodegradation: (Bioaccumulation test was carried out to tributyltin hydroxide) 1% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

307 • Bis-2-chloro-1-methylethylether 108-60-1

Sumformula of the chemical	ClCH2CH(CH3)OCH(CH3)CH2Cl	
Water solubility, mg/l	1800	(MITI 1992)
Boiling point, °C	185–190	(MITI 1992)
Log octanol/water coefficient, log Pow	2.11	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	6.4–12 < 5.2–9.0	6w, Cyprinus carpio, conc 0.4 mg/l 6w, Cyprinus carpio, conc 0.04 mg/l (MITI 1992)
Other information about mammals	Rat: inhalation: no effect level: 20 ppm (20 x 6 hr exposures) (Cage 1970).	
LC50 values to fishes, mg/l	71.2	48hr, Oryzias latipes (MITI 1992)

308 • Bisidin

14437-17-3

Synonyms	2-Chloro-3(4-chlorophenyl)-methylpropionate	
Use	Herbicide.	
State and appearance	Colourless to light-brown liquid.	
Specific gravity (water=1)	1.3	at 20/4 °C
Water solubility, mg/l	400	at 20 °C
LD50 values to mammals in oral exposure, mg/kg	1190–1390	orl-rat (Anon. 1976)
LD50 values to mammals in non-oral exposure, mg/kg	1273	skn-rat (Anon. 1976)
LC50 values to fishes, mg/l	1.1	96hr, Rasbora heteromorpha (Tooby et al. 1975)

309 • Blasticidin-S

2079-00-7

Use	Fungicide.	
LC50 values to crustaceans, mg/l	> 40	act, Daphnia pulex (Nishiuchi & Hashimoto 1967)
LC50 values to fishes, mg/l	40	48hr, Cyprinus carpio (Nishiuchi & Hashimoto 1967)

310 • Boric acid

10043-35-3

LC50 values to crustaceans, mg/l	133	48 hr, Daphnia magna (Gersich et al. 1984)

311 • Boron and boron compounds

7440-42-8

Molecular weight	10.81	
Effects on plants	In a micro-plot experiment 1.5 ppm boron in the irrigation water was toxic for wheat after the 3rd irrigation when 1.53 ppm B level in the soil solution was attained and B concentration in the plant tissue increased to 58 ppm (Chauhan & Powar 1978).	
LC50 values to fishes, mg/l	70.1	28 d, Salmo gairdneri (Birge et al. 1980)

312 • Boron oxide

1303-86-2

Synonyms	Boric anhydride Boron trioxide	
Sumformula of the chemical	B2O3	
Molecular weight	69.62	
LD50 values to mammals in oral exposure, mg/kg	3163	orl-mus (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	1868	ipr-mus (Sweet 1987)
Health effects	Skin and eye irritation data: skin, rabbit, 1000 mg; eye, rabbit, 50 mg (Sweet 1987).	

313 • Branched sodium alkyl benzenesulfonate; * C10 ~ C15

Synonyms	Sodium alkyl (branched type, C = 10-15) benzenesulfonate
Water solubility, mg/l	> 100 MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factorfishes	2.5–4.4 6w, Cyprinus carpio, conc 0.25 mg/l < 3.3–6.2 6w, Cyprinus carpio, conc 0.025 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	32.6 48hr, Oryzias latipes (MITI 1992)

314 • Bromacil

314-40-9

Synonyms	5-Bromo-3-sec-butyl-6-methyluracil 5-Bromo-6-methyl-3-(1-methylpropyl)uracil
Use	Herbicide used to control a wide range of grasses and broad-leaf weeds.
Melting point, °C	158–159
Log soil sorption coefficient, log Kom	1.86 (Sabljic 1987)
Photochemical degradation in water	Aqueous reactions: photo decomposition: the action of 4 months of sunlight on dilute (1–10 ppm) aqueous solutions of bromacil resulted in the formation of only one detectable photo product, 5-bromo-6-methyluracil in very low yield. The N-dealkylated photo product proved to be much less stable toward sunlight wavelengths, forming principally 6-methyluracil (Moilanen & Crosby 1974).
Half-life in soil, days	350 (Li et al. 1990)
LD50 values to mammals in oral exposure, mg/kg	5200 orl-rat (Anon. 1976)
Effects on plants	ED50 value for Brassica nigra in soil: < 0.01 mg/kg; (ED50 = the dose that reduces test plant fresh weight by 50%) (Angemar et al. 1984). 1.0 kg/ha bromacil was applied with a sprayer 24 days after seeding to lambs-quarters (Chenopodium album L.) in the 3 to 4-leaf stage —atrazine-suscepti-ble plants (seeds) were killed and there was a decrease in shoot growth and plant number of atrazine-resistant plants (Jensen et al. 1977).
LC50 values to fishes, mg/l	71 48hr, Lepomis macrochirus 75 48hr, Salmo gairdneri 164 48hr, Cyprinus carpio (Pesticide Manual 1983) 185 1d, Pimephales promelas 182 4d, Pimephales promelas 167 7d, Pimephales promelas (Call et al. 1987)
Effects on the physiology of water organisms	Pimephales promelas; 1 mg/l, 64 days; growth effect: measurable change in length and/or weight) (Call et al. 1987).

B

315 • 4-Bromo-2,5-dichlorophenol 1940-42-7

Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).

316 • 2-Bromo-4-nitrophenol 5847-59-6

Other information about water organisms	Fish: larvae of a sea lamprey: LD100 = 5 mg/l rainbow trout: LD10 = 13 mg/l brown trout: LD10 = 11 mg/l (McKee & Wolf 1963).

317 • 4-Bromoacetanilide 103-88-8

Sumformula of the chemical	C8H8BrNO
Log soil sorption coefficient, log Kom	1.71 (Sabljic 1987)

318 • 4-Bromoaniline 106-40-1

Synonyms	p-Bromoaniline 4-Bromobenzeneamine
Sumformula of the chemical	C6H6BrN
Use	Azo dye manufacturing, preparation of dihydroquinazolines (with formaldehyde).
State and appearance	Colourless, rhombic crystals.
Melting point, °C	66
Log soil sorption coefficient, log Kom	1.72 (Sabljic 1987)
Other physicochemical properties	Soluble in alcohol and ether; insoluble in cold water.

319 • Bromobenzene 108-86-1

Synonyms	Phenylbromide	
Sumformula of the chemical	C6H5Br	
Use	Solvent (fats, waxes, or resins); intermediates in specialty organic chemicals synthesis; additive to motor oil and fuels.	
Odour	Odour thresholds:	30.5 mg/m³ recognition 1.7–2.1 mg/m³ (Verschueren 1983).
Molecular weight	157.02	
Specific gravity (water=1)	1.5	at 15/15 °C
Vapour density (air=1)	5.41	
Conversion factor, 1 ppm in air=	6.53	mg/m³
Conversion factor, 1 mg/m³ in air=	0.15	ppm

B

Vapour pressure, mmHg	3.3	at 20 °C
Water solubility, mg/l	500 446 100	at 20 °C at 30 °C (MITI 1992)
Melting point, °C	-30.6	(MITI 1992)
Boiling point, °C	156.2	(MITI 1992)
Log octanol/water coefficient, log Pow	2.99 2.99 3.05	at 20 °C (Anon. 1986) (Sangster 1989) (MITI 1992)
Henry's law constant, Pa x m³/mol	211.4	calc. ((Yaws et al. 1991))
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).	
Bioconcentration factor, fishes	8.8–34 12–33	6w, Cyprinus carpio, conc 0.05 mg/l 6w, Cyprinus carpio, conc 0.005 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
Mutagenicity	Mutagenicity in the Salmonella test: none; < 0.01 revertant colonies/nmol; < 70 revertant colonies at 0.75 mg/plate (McCann et al. 1975).	
LC50 values to fishes, mg/l	6.8	48hr, Oryzias latipes (MITI 1992)
Other information	Man caused sources (water and air): general lab use; used as solvent; discharge of waste motor oils to water; road surface runoff.	

320 • Bromochloride 13863-41-7

Synonyms	Bromine chloride	
Molecular weight	115.36	
LC50 values to crustaceans, mg/l	0.10–0.21 0.10–0.21	48 hr, Crassostrea virginica (Roberts & Gleeson 1978) 48 hr, Acartia tonsa (Roberts & Gleeson 1978)
LC50 values to fishes, mg/l	0.21–0.23 0.21–0.23 0.21–0.23 0.6	96 hr, Medinia medinia (Roberts & Gleeson 1978) 96 hr, Breevortia tyranus (Roberts & Gleeson 1978) 96 hr, Leistomus canthurus (Roberts & Gleeson 1978) 96 hr, Palaemonetes spp. (Burton & Margrey)

321 • Bromochloromethane 74-97-5

Water solubility, mg/l	14000	(MITI 1992)
Melting point, °C	< -55	(MITI 1992)
Boiling point, °C	68–69	(MITI 1992)

Total degradation in water	Biodegradation: 0–12% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	1.7–3.5 < 2.1–2.9	6w, Cyprinus carpio, conc 1 mg/l 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	338	48hr, Oryzias latipes (MITI 1992)

322 • Bromocyanide 506-68-3

Synonyms	Cyanogen bromide	
Use	Organic synthesis; parasiticide; fumigating composition; rat exterminants.	
State and appearance	Crystals.	
Odour	Penetrating odour.	
Molecular weight	105.93	
Specific gravity (water=1)	2.015	at 20/4 °C (Verschueren 1983)
Vapour pressure, mmHg	100	at 22.6 °C (Verschueren 1983)
Melting point, °C	49–51	(Verschueren 1983)
Boiling point, °C	61–62	(Verschueren 1983)
Other physicochemical properties	Slowly decomposed by cold water.	
LC50 values to fishes, mg/l	0.24 0.47	96 hr, Lepomis macrochirus 96 hr, Menidia audens (Dawson et al. 1977)

323 • Bromocyclohexane 108-85-0

Sumformula of the chemical	C6H11Br	
Log octanol/water coefficient, log Pow	3.2	(Sangster 1989)
EC50 values to algae, mg/l	2.5	rpd, act, 24 hr, Chlorella pyrenoidosa (Canton & Wegman 1983)
EC50 values to crustaceans, mg/l	2.3	srv, 48 hr, Daphnia magna (Canton & Wegman 1983)

324 • Bromodichloromethane 75-27-4

Sumformula of the chemical	CHBrCl2
Use	Fire extinguisher fluid ingredient; solvent (fats, waxes, resins); synthesis intermediate; heavy liquid for mineral and salt separations.
State and appearance	Colourless liquid,
Molecular weight	163.8

Specific gravity (water=1)	1.971	at 25/25 °C
Water solubility, mg/l	4500	(Mabey et al. 1982)
Melting point, °C	-57.1	(Suntio et al. 1988)
Boiling point, °C	90	
Log octanol/water coefficient, log Pow	2.1 1.88	(Mabey et al. 1982) (Callahan et al. 1979)
Henry's law constant, Pa x m³/mol	242	calc. (Suntio et al. 1988)
Other information	Man caused sources (water and air): results from chlorination of finished water; use of fire extinguishers, lab use.	

325 • Bromoethane 74-96-4

Synonyms	Ethylbromide	
Sumformula of the chemical	C2H5Br	
Use	Solvent.	
Water solubility, mg/l	9100	20 °C
Melting point, °C	-125.5	(MITI 1992)
Boiling point, °C	38.4	760 mmHg (MITI 1992)
Log octanol/water coefficient, log Pow	1.61 1.51	(Sangster 1989) (MITI 1992)
Henry's law constant, Pa x m³/mol	751	calc. (Yaws et al. 1991)
Volatilization	Relative volatility (nBuAc=1) = 46.19	
Total degradation in water	Biodegradation: 13–45% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

326 • Bromoform 75-25-2

Synonyms	Tribromomethane	
Sumformula of the chemical	CHBr3	
Use	Pharmaceutical manufactures; ingredient in fire-resistant chemicals; gage fluid; heavy liquid in solid separations based on differences in specific gravity, geological assaying, solvent for waxes, greases and oils.	
State and appearance	Colourless liquid.	
Odour	Characteristic; chloroform like, sweetish (Patty 1967). Odour threshold in water; detection: 0.3 mg/kg (Verschueren 1983).	
Molecular weight	252.77	
Specific gravity (water=1)	2.89	at 20/4 °C
Vapour density (air=1)	8.7	
Conversion factor, 1 ppm in air=	10.34	mg/m³

Conversion factor, 1 mg/m³ in air=	0.0966	ppm
Vapour pressure, mmHg	5.6	at 25 °C
Water solubility, mg/l	3190 2001	at 20 °C (MITI 1992)
Melting point, °C	6–7	
Boiling point, °C	149.5	(MITI 1992)
Log octanol/water coefficient, log Pow	2.4	(MITI 1992)
Aerobic degradation in sediment	Biodegradation: 0% by GC analysis period: 28d substance: 100 mg/l sludge 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	7.1–21 7.7–19	6w, Cyprinus carpio, conc 0.1 mg/l 6w, Cyprinus carpio, conc (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	1400 1147	orl-mus orl-rat (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	9274 414 1820	ipr-mam ipr-rat scu-mus (Sweet 1987)
LC50 values to mammals in inhalation exposure, mg/m³	12100	ihl-mam (Sweet 1987)
LDLo values to mammals in oral exposure, mg/kg	143	orl-hmn (Sweet 1987)
LDLo values to mammals in non-oral exposure, mg/kg	410	scu-rbt (Sweet 1987)
LCLo values to mammals in inhalation exposure, mg/kg	45	ihl-rat, 4hr (Sweet 1987)
TDLo values to mammals in non-oral exposure, mg/kg	1100	ipr-mus, tumorigenic (Sweet 1987)
LC50 values to crustaceans, mg/l	46	48 hr, Daphnia magna (LeBlanc 1980)
LC50 values to fishes, mg/l	29 18 40.4	96 hr, Lepomis macrochirus (Buccafusco et al. 1981) 96 hr, Cyprinodon variegatus (Heitmuller et al. 1981) 48hr, Oryzias latipes (MITI 1992)
LOEC values to fishes, mg/l	24	Cyprinodon variegatus (Ward & Parrish 1980)
Other information about water organisms	Larvae of eastern oyster (Crassostrea virginica): LD50, 48 hr: 1 mg/l, initial conc., static test (after 48 hr only approximately 30% of original conc. was still present (Verschueren 1983).	

B

327 • 4-Bromonitrobenzene 586-78-7

Sumformula of the chemical	C6H4BrNO2	
Log soil sorption coefficient, log Kom	2.18	(Sabljic 1987)

328 • o-Bromonitrobenzene 577-19-5

Chemical oxygen demand, g O2/g	1.11	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g O2/g	0.1	5 days, Bridie et al.1979
LC50 values to fishes, mg/l	46	24 hr, Carassius auratus (Bridie et al. 1979)

329 • 2-Bromophenol 95-56-7

Synonyms	o-Bromophenol	
Molecular weight	173.02	
Specific gravity (water=1)	1.49	at 20/4 °C
Water solubility, mg/l	> 1000	(MITI 1992)
Melting point, °C	5.6	(MITI 1992)
Boiling point, °C	194	(MITI 1992)
Log octanol/water coefficient, log Pow	2.29	(MITI 1992)
Total degradation in soil	Biodegradation: decomposition rate in soil suspensions: 14 days for complete disappearance (Woodcock 1971).	
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	20–33 23–41	6w, Cyprinus carpio, conc 0.03 mg/l 6w, Cyprinus carpio, conc 0.003 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
Effects on wastewater treatment	Waste water treatment: degradation by Pseudomonas: 200 mg/l at 30 °C ring disruption: parent: 100% in 85 hr mutant: 100% in 14 hr (Verschueren 1983).	
LC50 values to fishes, mg/l	16	48 hr, Oryzias latipes (MITI 1992)
Other information about water organisms	Algae: Chlorella pyrenoidosa: 78 mg/l: toxic (Jones 1971).	

330 • 3-Bromophenol

591-20-8

Synonyms	m-Bromophenol	
Odour	Odour threshold; recognition: 0.000007 mg/m³ (Kendall et al. 1968).	
Molecular weight	173.02	
Water solubility, mg/l	23000	(MITI 1992)
Melting point, °C	30.6	(MITI 1992)
Boiling point, °C	236	(MITI 1992)
Log octanol/water coefficient, log Pow	2.78	(MITI 1992)
Total degradation in soil	Biodegradation: decomposition rate in suspended soils: > 72 days for complete disappearance (Woodcock 1971).	
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	4.1–10 < 16	6w, Cyprinus carpio, conc 0.06 mg/l 6w, Cyprinus carpio, conc 0.006 mg/l (MITI 1992)
LC50 values to fishes, mg/l	11	48 hr, Oryzias latipes (MITI 1992)
Other information about water organisms	Fish: larvae of sea lamprey: LD100: 3 mg/l rainbow trout: LD10: 5 mg/l brown trout: LD10: 5 mg/l (McKee & Wolf 1963). Algae: Chlorella pyrenoidosa: 36 mg/l: toxic (Jones 1971).	

331 • 4-Bromophenol

106-41-2

Synonyms	p-Bromophenol	
Molecular weight	173.02	
Specific gravity (water=1)	1.84	at 15 °C
Water solubility, mg/l	14200 14000	at 15 °C (MITI 1992)
Melting point, °C	64	(MITI 1992)
Boiling point, °C	235–236	(MITI 1992)
Log octanol/water coefficient, log Pow	2.59 1.1	 (MITI 1992)
Log soil sorption coefficient, log Kom	2.17 2.53	observed (Sabljic 1987) calculated (Sabljic 1987)
Total degradation in soil	Biodegradation: decomposition rate in soil suspensions: 16 days for complete disappearance (Woodcock 1971).	

Total degradation in water	Biodegradation: 0% by BOD substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	8.0–12 6w, Cyprinus carpio, conc 0.03 mg/l < 4.8–25 6w, Cyprinus carpio, conc 0.003 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
Other information about biodegradation	Degradation by Pseudomonas: 200 mg/l at 30 °C: ring disruption: parent: 87% in 85 hr mutant: 100% in 22 hr (Verschueren 1983).
LC50 values to fishes, mg/l	6.1 48 hr, Oryzias latipes (MITI 1992)
Other information about water organisms	Algae: Chlorella pyrenoidosa: toxic: 36 mg/l (Jones 1971).

332 • Bromophenoxim

13181-17-4

Synonyms	3,5-Dibromo-4-hydroxybenzaldehyde-o-(2',4'-dinitrophenyl)oxime Faneron Combi 500 FW *
Sumformula of the chemical	C13H7Br2N3O6
Products containing the chemical	Faneron Combi 500 FW: * Bromophenoxim 330 g/l * Terbutylazine 170 g/l (PESREG)
Use	Herbicide.
State and appearance	Cream-coloured, crystalline powder. (PESREG)
Molecular weight	461.02
Vapour pressure, mmHg	< 0.00000001, at 20 °C (PESREG)
Water solubility, mg/l	0.1 at 20 °C (PESREG)
Melting point, °C	196–197 (PESREG)
Mobility	In the soil column studies (sandy soil and silty loam, incubated 30 days and then rainfall 16 days, 12.5 mm daily) of bromophenoxim (2.5 kg/ha) 1.09 and 0.74% of the applied radioactivity were found in the column eluates (PESREG). The leaching behaviour of bromophenoxim (5.0 kg a.i./ha) was studied in the soil columns. 87.8% (a sandy soil), 97.6% (a silty loam), 85.0% (a sandy loam) and 87.0% (a pure sand) of applied radioactivity were retained in the upper 2 cm (PESREG). Leaching of bromophenoxim (C-14-dibromophenyl-labelled) was studied in the aged soil (2.5 kg a.i./ha, incubated 5 months, and then watered 393 ml/two days). 1.88% of applied radioactivity was recovered in the leachate (PESREG). Solubility in organic solvents hexane: 200 ppm isopropanol: 400 ppm benzene: 500 ppm (PESREG).
Photochemical degradation in water	Photolysis of bromophenoxim (1 ppm) was studied using a mercury arc as the source of light. Half-life was found 38 s. The degradation product (C-14-dinitrophenyl-labelled) was 2,4-dinitrophenol (PESREG).

Hydrolysis in water	The half-life of bromophenoxim (1-2 ppm) was 0.94 hr (pH 7, 70 °C). The major degradation product (C-14-dinitrophenyl-labelled) was 2,4-dinitrophenol. The degradation product (C-14-dibromophenyl-labelled) (at pH 7) was 3,5-dibromo-4-hydroxybenzaldoxime (PESREG).
Hydrolysis in acid	The half-lives of bromophenoxim (1-2 ppm) were 41.4 hr (pH 1, 70 °C) and 9.6 hr (pH 5, 70 °C). The major degradation product (C-14-dinitrophenyl-labelled) (at pH 1) was 2,4-dinitrophenol. The major degradation product (C-14-dibromophenyl-labelled) (at pH 1) was 3,5-dibromo-4-hydroxybenzonitrile (PESREG).
Hydrolysis in base	The half-lives of bromophenoxim (1-2 ppm) were 0.76 hr (pH 9, 70 °C) and < 0.3 min (pH 13, 70 °C). The major degradation product (C-14-dinitrophenyl-labelled) (at pH 13) was 2,4-dinitrophenol. The major degradation product (C-14-dibromophenyl-labelled) (at pH 13) was 3,5-dibromo-4-hydroxybenzonitrile (PESREG).
Aerobic degradation in soil	The half-life of bromophenoxim (C-14-dibromophenyl-labelled) in soil under aerobic conditions was 90.1 days. The primary extractable intermediates were 3,5-dibromo-4-hydroxybenzonitrile, 3,5-dibromo-4-hydroxybenzaldehyde and probably 3,5-dibromo-4-hydroxy-benzoisonitrile. 29.1% from applied radioactivity was liberated as carbon dioxide after 7 months (PESREG).
Aerobic degradation in water	The half-life of bromophenoxim (1.0 mg/l) was << 7 days in two aquatic model (river and pond, both 1% of sediment) systems. After 77 days metabolite 3,5-dibromo-4-hydroxybenzonitrile was found 67.3% (river) and 11.5% (pond) of applied radioactivity. The metabolite 3,5-dibromo-4-hydroxybenzamide was found after 77 days 4.4% (river) of applied radioactivity. The volatile radioactivity in form of 14CO2 were observed after 77 days 19.7% (river) and 51.8% (pond) of applied radioactivity (PESREG).
Total degradation in soil	The degradation in soil of bromophenoxim was investigated under two conditions (laboratory, field) using C-14-dibromophenyl and C-14-dinitrophenyl ring labelled herbicide. In the laboratory experiment 4% of (C-14-dibromophenyl-labelled)applied radioactivity was recovered as unchanged after 12 weeks. In the field (2 kg a.i./ha) experiment where both of the labelled varieties were applied less than 6% of the radioactivity was characterized as bromophenoxim after 16 weeks. Bromophenoxim (4.2 ppm) was incubated in soil (C-14-dibromophenyl-labelled). Appr. 40% of applied radioactivity was liberated as 14CO2 within 12 weeks. The degradation products (C-14-dibromophenyl-labelled) were found: 3,5-dibromo-4-hydroxybenzaldehyde, 3,5-dibromo-hydroxybenzonitrile, 3,5-dibromo-4-hydroxybenzamide and 3,5-dibromo-4-hydroxybenzoic acid. The degradation product (C-14-dinitrophenyl-labelled) was 2,4-dinitrophenol (PESREG).
Degradation and transformation products	C-14-dinitrophenyl-labelled: 2,4-dinitrophenol C-14-dibromophenyl-labelled: 3,5-dibromo-4-hydroxybenzaldoxime 3,5-dibromo 4-hydroxybenzonitrile 3,5-dibromo-4-hydroxybenzaldehyde 3,5-dibromo-4-hydroxybenzoic acid 3,5-dibromo-4-hydroxybenzamide (PESREG)
Metabolism in plants	Metabolism of bromophenoxim was studied in laboratory grown winter wheat after foliar application. Five weeks after the treatment 22.6% (C-14-dinitrophenol-labelled) and 30.23% (C-14-dibromophenol-labelled) of the radioactivity applied were recovered from treated plants (PESREG).
LD50 values to mammals in oral exposure, mg/kg	940 orl-mus (PESREG)
LD50 values to mammals in non-oral exposure, mg/kg	719 ipr-mus (PESREG) > 3000 idr-rat (PESREG)
LC50 values to mammals in inhalation exposure, mg/m³	> 242 6hr, ihl-rat (PESREG)

B

LD50 values to birds in oral exposure, mg/kg	2800 4000 5560	orl-bdw, Anas platyrhyncos orl-bdw, Coturnix virginianus orl-bdw, Coturnix japoniensis (PESREG)
Effects on microorganisms	The influence of bromophenoxim on soil (loamy sand, silt) microbes was determined by measuring soil respiration, ammonification and nitrification. Bromophenoxim showed a very slight inhibitory effect on soil respiration (averaged 7%) during 4 weeks. In a six weeks study bromophenoxim has no negative effect on the ammonification and nitrification process in the soil (PESREG).	
EC50 values to algae, mg/l	2.3 2.2	5d, grw, Scenedesmus subspicatus calc. 5d, grw, Scenedesmus subspicatus (PESREG)
LC50 values to crustaceans, mg/l	1.2	48hr, Daphnia magna (PESREG)
EC50 values to crustaceans, mg/l	1.6	24hr, imb, Daphnia magna (PESREG)
LC50 values to fishes, mg/l	0.18 0.18 0.09 0.088	96hr, Salmo gairdneri, OECD 203 96hr, calc. Salmo gairdneri 96hr, Cyprinus carpio, OECD 203 96hr, calc. Cyprinus carpio (PESREG)

333 • 4-Bromophenylphenylether 101-55-3

LC50 values to crustaceans, mg/l	0.36	48 hr, Daphnia magna (LeBlanc 1980)

334 • Bromophos 2104-96-3

Use	Active ingredient in insecticides.	
LC50 values to crustaceans, mg/l	0.0064	Daphnia pulex (Frear et al. 1967)
LC50 values to fishes, mg/l	0.5	Poecilia reticulata (Pesticide Manual 1983)
Other information about water organisms	LOEC 5.6 mg/l, srv, act, Colpidium campylum (Dive et al. 1980).	

335 • Bromophos-ethyl 4824-78-6

Use	Insecticide.	
LC50 values to fishes, mg/l	0.14–0.24 > 0.4	96 hr, Poecilia reticulata (Pesticide Manual 1983) 96 hr, Salmo gairdneri (Pesticide Manual 1983)

336 • β-Bromostyrene 103-64-0

Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).

B

337 • Bromoxynil
1689-84-5

Synonyms	3,5-Dibromo-4-hydroxybenzonitrile	
Sumformula of the chemical	C7H3Br2NO	
Use	Herbicide.	
Molecular weight	276.93	
LD50 values to mammals in oral exposure, mg/kg	190 63	orl-rat orl-gpg (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	200	orl-dck (Lewis & Sweet 1984)
LC50 values to crustaceans, mg/l	0.011	act, Daphnia magna (Kenaga 1979)
LC50 values to fishes, mg/l	0.05 0.46	act, Salmo gairdneri (Kenaga 1979) 48hr, Carassius auratus (Pesticide Manual 1983)

338 • Bromoxynil octanoate
1689-99-2

Synonyms	3,5-Dibromo-4-octanoyloxy-benzonitrile 2,6-Dibromo-4-cyanophenyl octanoate 3,5-Dibromo-4-hydroxyphenyl cyanide	
Sumformula of the chemical	C15H17Br2NO2	
State and appearance	Cream, waxy solid.	
Molecular weight	403.15	
Melting point, °C	45–46	
Hydrolysis in base	Bromoxynil octanoate is hydrolyzed to bromoxynil at pH > 9 (Pesticide Manual 1987).	
LD50 values to mammals in oral exposure, mg/kg	250 245 2000	orl-rat (Sweet 1987) orl-mus (Sweet 1987) orl-rbt (Sweet 1987)
Effects on bees	Spray of 3.4 g bromoxynil octanolate/l showed no contact toxicity to honeybees (Pesticide Manual 1987).	
Effects on plants	The isooctyl ester of bromoxynil was applied with a sprayer at 0.28 kg/ha → slight leaf burn and epinastic responses were noted in red clover (Trifolium pratense) (Darwent & Pankiw 1976).	
LC50 values to fishes, mg/l	0.15	48hr, Salmo gairdneri (Pesticide Manual 1987)

339 • Brucine
357-57-3

Synonyms	Dimethoxystrychnine
Use	Medicine; denaturing alcohol; lubricant additive.
State and appearance	White crystalline alkaloid; very bitter taste.
Molecular weight	394.45
Melting point, °C	178
Other information about degradation	Impact on biodegradation processes: at 100 mg/l no inhibition of NH3 oxidation by Nitrosomonas sp. (Hockenbury & Grady 1977).

Brucin

LC50 values to fishes, mg/l	36 20	96 hr, Lepomis macrochirus 96 hr, Menidia beryllina (Dawson et al. 1977)

340 • Busan 25 * 37301-44-3

Active ingredients	2-(thiocyanomethylthio)-benzothiazole * 13%; 2-hydroxypropylmethanethiolsulfonate * 11.7%	
Use	Microbicide.	
LC50 values to fishes, mg/l	0.42 0.57 1	96hr, Rasbora heteromorpha 48hr 24hr (Tooby et al. 1975)

341 • Busan 70 * 21564-17-0

Active ingredients	Butanethiol sulfonate	
Use	Microbicide.	
LC50 values to fishes, mg/l	0.43	96hr, Rasbora heteromorpha (Tooby et al. 1975)

342 • Busan 72 * 21564-17-0

Active ingredients	2-(thiocyanomethylthio)benzothiazole * 60%	
Use	Microbicide.	
Water solubility, mg/l	33	(MITI 1992)
Melting point, °C	< -10	(MITI 1992)
Boiling point, °C	> 149	(MITI 1992)
Log octanol/water coefficient, log Pow	3.3	(MITI 1992)
Total degradation in water	Biodegradaation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 14–20 < 153–268	8w, Cyprinus carpio, conc 0.002 mg/l 8w, Cyprinus carpio, conc 0.0002 mg/l (MITI 1992)
LC50 values to fishes, mg/l	0.036 98.9	96hr, Rasbora heteromorpha (Tooby et al. 1975) 48hr, Oryzias latipes (MITI 1992)

343 • Busan 76 * 27983-69-3

Active ingredients	β-cyanoethyl-2,3-dibromo-propionate * 60%	
Use	Microbicide.	
LC50 values to fishes, mg/l	0.31	96hr, Rasbora heteromorpha (Tooby et al. 1975)

344 • Busan 77 *

31512-74-0

Active ingredients	Quarternary ammonium compound.	
Use	Slimicide; microbicide.	
LC50 values to fishes, mg/l	0.17 0.39	96hr, Rasbora heteromorpha 48hr (Tooby et al. 1975)

345 • Busan 881 *

8070-47-1

Active ingredients	Disodiumcyanodithioimidocarbonate * 12.7%; Potassium-N-methyldithiocarbamate * 17.5%	
Use	Slimicide.	
LC50 values to fishes, mg/l	0.65 1.1	48 hr, Rasbora heteromorpha 24 hr, R. heteromorpha (Alabaster 1969)
	1.7	96 hr, Lepomis macrochirus (Landner et al. 1976)

346 • Busan 90 *

2491-38-5

Active ingredients	2'-bromo-4'-hydroxyacetophenone * 30%	
Use	Slimicide	
LC50 values to crustaceans, mg/l	17	96 hr, Asellus (Landner et al. 1973)
LC50 values to fishes, mg/l	0.6 4.5 0.8	24 hr, Rasbora heteromorpha 24 hr, Poecilia reticulata 72 hr, Anodonta cygnea (Landner et al.1973)
	1.85	24 hr, Phoxinus phoxinus (Niemi 1971)
	1.8 1.5	24 hr, Rasbora heteromorpha 48 hr, R. heteromorpha (Alabaster 1969)

347 • Butachlor

23184-66-9

EC50 values to algae, mg/l	0.04	rpd, Chlamydomonas reinhardii (Lee & Hong 1982)

348 • 1,3-Butadiene

106-99-0

Synonyms	Vinylethylene Divinyl Bivinyl Pyrrolylene Biethylene Erythrene
Sumformula of the chemical	CH2=CH-CH=CH2
Use	Principally in styrene-butadiene rubber; in latex paints; resins; organic intermediate.

State and appearance	Colourless gas.	
Odour	Characteristic: quality: undefined. Hedonic tone: unpleasant to neutral. Odour index (100% recognition): 770000 (Hellman & Small 1974). Quality: undefined Hedonic tone: unpleasant to neutral Threshold odour concentration: absolute: 0.45 ppm 50% recognition: 1.1 ppm 100% recognition: 1.3 ppm Odour index 100% recognition: 769 230 (Hellman & Small 1974)	
Molecular weight	54.09	
Specific gravity (water=1)	0.6211	at 20 °C liquified
Vapour density (air=1)	1.87	
Conversion factor, 1 ppm in air=	2.25	mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.45	ppm
Vapour pressure, mmHg	1840 856	20 °C -1.5 °C (Boublik et al. 1984)
Water solubility, mg/l	735 735	at 20 °C at 25 °C (McAuliffe 1966)
Melting point, °C	-108.9	
Boiling point, °C	-4.41 -4.5	 at 760 mmHg (Howard I 1990)
Log octanol/water coefficient, log Pow	1.99 1.99	(Hansch & Leo 1985) (Sangster 1989)
Henry's law constant, Pa x m^3/mol	7220	calc. (Yaws et al. 1991)
Volatilization	Using the Henry's Law constant, the estimated half-life for evaporation of 1,3-butadiene from a river 1 m deep with with a 1 m/sec current and a 3 m/sec wind is 3.8 hours. (Lyman et al. 1982) Due to its low boiling point, 1,3-butadiene would be expected to rapidly evaporate from soils (Howard I 1990).	
Adsorption/desorption	The range of estimated adsorption coefficients for 1,3-butadiene from the soils and sediments is 72–228 based on its octanol/water partition coefficient or its water solubility. It would therefore not be expected to appreciably adsorb in soils and sediments (Lyman et al. 1982) (Howard 1989).	
Photochemical degradation in air	The estimated half-life for 1,3-butadiene due to photo oxidation with hydroxyl radicals is 3.1 hours. (Lyman et al. 1982) Stable reaction products of photo oxidation are acetaldehyde and acrolein. (Graedel 1978)	

Other reactions in atmosphere	Estimated lifetime under photochemical smog conditions in S.E.England: 0.48 hr (Darnall et al. 1976). Within 5 hours, 100% degradation of 1,3-butadiene was observed in a smog chamber artificially irradiated and in 6 hours in Los Angeles air irradiated with sunlight. (Yanagihara et al. 1977) (Kopcynski et al. 1972) When 1,3-butadiene was irradiated with black lights in Riverside, CA air, 100% degradation was observed within 8 hours with heavy haze and within 4 hours with light haze. (Stephens & Burleson 1967) The reaction with nitrate radicals has been recognized as an important nighttime sink for some chemicals. The half-life for the reaction of 1,3-butadiene is 15 hr. (Atkinson et al. 1984)
Other information about degradation	Screening tests suggest that 1,3-butadiene may be biodegradable in the environment with 1,2-epoxybutene being a potential product. (Hou et al. 1983)
Health effects	Man: irritation of the respiratory system; 10000 ppm, 1 min.; slight irritation of the eyes and upper respiratory tract, no other effects: 8000 ppm, 8 hr (Verschueren 1983, Patty 1967).
LC50 values to fishes, mg/l	71.5 24 hr, pinperch (Jones 1971)

349 • n-Butane

106-97-8

Sumformula of the chemical	CH3CH2CH2CH3
State and appearance	Colourless gas.
Odour	Threshold odour concentration: 12100 mg/m³ = 4960 ppm not detectable: < 5000 ppm (Patty 1967) recognition: 6160 mg/m³ (Verschueren 1983) 3000 mg/m³ (Laffort & Dravnieks 1973) 5.5 ppm (Verschueren 1983).
Molecular weight	58.14
Specific gravity (water=1)	0.6 liquified
Vapour density (air=1)	2.01
Conversion factor, 1 ppm in air=	2.42 mg/m³
Conversion factor, 1 mg/m³ in air=	0.41 ppm
Vapour pressure, mmHg	1823 at 25 °C
Water solubility, mg/l	61 at 20 °C 30 at 15 °C 21 at 38 °C
Melting point, °C	-135– -138
Boiling point, °C	-1
Photochemical degradation in air	Estimated lifetime under photochemical smog conditions in S.E. England: 15 hr (Verschueren 1983, Stuhl 1973).
Total degradation in water	Incubation with natural flora in the groundwater – in presence of the other components of high-octane gasoline (0.100 ml/l): biodegradation: 0% after 192 hr at 13 °C (initial conc. 0.00063 ml/l (Jamison et al. 1976).
Health effects	Man: drowsiness, no other effects; 10000 ppm, 10 min (Patty 1967).

B

350 • 1,4-Butanediol

110-63-4

Synonyms	Tetramethyleneglycol 1,4-Dihydroxybutane
Sumformula of the chemical	(CH2CH2OH)2
Molecular weight	90.12
Specific gravity (water=1)	1.02 at 20/4 °C
Water solubility, mg/l	> 100 000(MITI 1992)
Melting point, °C	20 (MITI 1992)
Boiling point, °C	235 (MITI 1992)
Total degradation in water	Biodegradation: 74–96% by BOD period: 14d substance: 100 mg/l sludge 30 mg/l (MITI 1992).

351 • 1-Butanol

71-36-3

Synonyms	1-Butyl-alcohol Butanol-1 Normal butyl alcohol 1-Hydroxybutane Normal-propyl carbinol Butyric alcohol NBA Butan-1-ol Butyl alcohol n-Butylalcohol Propylcarbinol n-Butanol
Sumformula of the chemical	C4H100
Use	1-butanol is used as an ingredient in perfumes and flavours (Mellan 1950) and of: hop, lipid-free protein from egg yolk (Meslar & White 1978), natural flavouring materials and vegetable oils, phenols, and oligosaccharides from plant tissue (Sodini & Canella 1977), and as a solvent in removing pigments from moist curd leaf protein concentrate (Bray & Humbries 1978).1-butanol is also used as: an extractant in the manufacture of antibiotics, hormones, and vitamins (Mellan 1950, Doolittle 1954, Yamazaki & Kato 1978), and of rhenium (Gukosyan et al. 1979); a solvent for paints, coatings, natural resins, gums, synthetic resins, dyes, alkaloids, and camphor (Mellan 1959, Doolittle 1954); a cleanser for moulded contact lenses (Mitazani et al. 1978); an intermediate in the manufacture of butyl acetate, dibutyl phthalate, and dibutyl sebacate (Mellan 1950, Doolittle 1954) as well as of the esters of herbicides (Monich 1968). Other miscellaneous applications of 1-butanol are as a swelling agent in textiles, as a component of brake fluids, cleaning formulations, degreasers (Monich 1968, Sitanov et al.1979), and repellents (Zaikina et al.1978); and as a component of ore flotation agents (Monich 1968), of protective coatings for glass objects (Artigas Gimenez et al. 1979) and of wood-treating systems (Amundsen et al. 1979). Mixed with xylene, it is used to produce a glass substitute (Ferri 1979). It is also used as an additive to increase the fineness of ground cement (Tavlinova & Dovyborova 1979) and as a solvent in the purification of polyolefins (Takeuchi et al. 1978). It may be liberated during photographic processing operations. A further use of 1-butanol is as a flavouring agent in bu tter, cream, fruit, liquor, rum, and whisky. Other foods in which it is used include: Beverages, ice cream and ices, candy, baked goods, cordials and cream (Hall & Oser 1965).

State and appearance	Colourless liquid.	
Odour	Characteristic; rancid sweet. Hedonic tone: neutral to pleasant. Odour threshold approximately 3.078 mg/m³. At a concentration of 20 mg/l, butanol gives a strong unpleasant odour to drinking water. The odour threshold is 1 mg/l (Nazarenko 1969). Threshold for unadapted panellists: 50 ppm Threshold after adaption with pure odourant: 10000 ppm Distinct odour: 48 mg/m³ = 16 ppm (Verschueren 1983). In water: 20% of the population still able to detect odour at 1.5 ppm 10% of the population still able to detect odour at 1.2 ppm 1% of the population still able to detect odour at 0.44 ppm 0.1% of the population still able to detect odour at 0.16 ppm (Lillard et al. 1975). Quality: rancid, sweet Hedonic tone: neutral to unpleasant Threshold odour concentration: absolute: 0.30 ppm 50% recognition: 1.0 ppm 100% recognition: 2.0 ppm Odour index 100% recognition: 2 630 (Hellman & Small 1974).	
Molecular weight	74.12	
Specific gravity (water=1)	0.81	at 20/4 °C
Vapour density (air=1)	2.55	
Density, kg/m³	809–811	
Conversion factor, 1 ppm in air=	3.078	mg/m³
Conversion factor, 1 mg/m³ in air=	0.325	ppm
Vapour pressure, mmHg	4.4 7.024 10	20 C 25 C (Daubert & Danner 1985) 30 C
Water solubility, mg/l	77000	(Barton 1984)
Melting point, °C	-89.5	
Boiling point, °C	117.2	
Log octanol/water coefficient, log Pow	0.8 0.88 0.84	Anon. 1986 (Hansch & Leo 1985) (Sangster 1989)
Henry's law constant, Pa x m³/mol	0.564	(Mackay & Yeun 1983)
Volatilization	Relative volatility (nBuAc=1) = 0.47	
Mobility	Using a measured log octanol/water partition coefficient of 0.88, a soil sorption coefficient (Koc) of 71.6 was estimated (Lyman et al. 1982). A Koc of this magnitude suggests that n-butanol will be moderately to highly mobile in the soil (Kenaga 1980).	
Chemical oxygen demand, g 02/g	2.46	5 days (Bridie et al. 1979)

Biochemical oxygen demand, g 02/g	1.71 5 days (Bridie et al. 1979)
Total degradation in soil	When released to soil n-butanol is expected to leach to ground water or to biodegrade. Volatilization from the soil surface may also occur (Howard II 1990).
Total degradation in water	In water, n-butanol is expected to biodegrade. Volatilization from the water surface is expected to occur with estimated half-lives of 2.4 hr, 3.9 hr and 125.9 days in streams, rivers and lakes (Lyman et al. 1982).
Other information about degradation	Impact on biodegradation processes: 50% inhibition of NH3 oxidation in Nitrosomonas at 8200 mg/l (Verschueren 1983). A 3 ppm solution of n-butanol was incubated in river water at 18–19 °C exerted a biological oxygen demand (BOD) of about 4.5 ppm after about 4 days (Hammerton 1955). After 5 days 33% of the theoretical BOD was exerted in a solution of n-butanol containing an inoculum from polluted surface water (Dore et al. 1975). In a batch system, n-butanol was dissolved to give a concentration corresponding to a chemical oxygen demand (COD) of 200 mg/l (Pitter 1976). Sufficient adapted activated sludge was added to make the dry matter of the inoculum 100 mg/l and the system was incubated at 20 °C. Under these conditions a total of 98.9% of the initial n-butanol was removed at a rate of 84.0 mg COD/g hr (Hammerton 1955). After 5 days incubation at 20 °C, 66% of the theoretical oxygen demand had been exerted in a BOD test (Bridie 1979).
Other information about bioaccumulation	1-butanol does not bioaccumulate (Chiou et al. 1977).
LD50 values to mammals in oral exposure, mg/kg	3400 orl-rbt (Münch & Schwartze 1925) 2100 orl-rat (Jenner et al. 1964) 800–1200 orl-rat (Purchase 1969) 3500 orl-rbt (Münch 1972) 1200 orl-hamster (Dubina & Maksikov 1976) 700 orl-rat (NIOSH 1977a 2680 orl-mus (Rumyanstev et al. 1979) 4360 orl-rat 4250 orl-rbt (Patty 1967) 710 orl-rat
LD50 values to mammals in non-oral exposure, mg/kg	240 ivn-cat (Macht 1920) 4200 skn-rbt (Egorov 1972) 5300 skn-rbt 5000 mus-cat (Patty 1982)

Other information about mammals	1-butanol is readily absorbed through the skin, lungs, and gastrointestinal tract. In animals, 1-butanol is rapidly metabolized by alcohol dehydrogenase to the corresponding acid, via the aldehyde, and to carbon dioxide, which is the major metabolite. 1-butanol is slightly toxic to mammals, markedly irritating to the eyes and moderately irritating to the skin. The primary effects from exposure to vapour for short periods are various levels of irritation of the mucous membranes and central nervous system depression. Its potency for intoxication is approximately 6 times that of ethanol. A variety of investigations have indicated non-specific membrane effects of 1-butanol. Effects of repeated inhalation exposure in animals include pathological changes in the lungs, degenerative lesions in the liver and kidneys, and narcosis. However, from the animal studies available, it is not possible to determine a no-observed-adverse-effect- level. 1-butanol has been found to be non-mutagenic. No adequate data are available on carcinogenicity, teratogenicity, or effects on reproduction (WHO 1987). Mouse: inhalation: no effect: 1650 ppm, 420 min. (Patty 1967).
Health effects	In man, 1-butanol, in the liquid or vapour phase can c ause moderate skin irritation and severe eye irritation manifested as a burning sensation, lachrymation, blurring of vision, and photophobia. Ingestion of the liquid or inhalation of the vapour may result in headache, drowsiness, and narcosis. The occurance of vertigo under conditions of severe and prolonged exposure to vapour mixtures of 1-butanol and isobutanol has been reported. From this study it was not possible to attribute to vertigo to a single cause. The symptoms were reversible when exposure ceased. The minimal information available suggest that occupational human exposure to air concentrations below 307.8 mg/m³ is not associated with any adverse symptoms. However, studies on human volunteers indicate that the light sensitivity of dark-adapted eyes and electrical activity of the brain may be influenced by air concentrations as low as 0.092 mg/m³. Man: mild irritation of nose, throat, and eyes: 25 ppm pronounced irritation: 50 ppm (Patty 1967).
Mutagenicity	Mutagenicity in the Salmonella test: none: < 0.0005 revertant colonies/nmol < 70 revertant colonies at 10 mg/plate (McCann et al. 1975).
LD50 values to birds in oral exposure, mg/kg	< 2500 orl-Sturnus vulgaris (Schafer et al. 1983)
Effects on amphibia	Threshold for narcosis: 2820 mg/l, Rana sp. (Münch 1972)
Effects on plants	Seed germination in lettuce (Lactuca sativa) was inhibited by 50% at a concentration of 1-butanol of 390 mg/l (Reynolds 1977). Seed germination in cucumber (Cucumis sativus) was inhibited at 2500 mg/l (Smith & Siegal 1975). 1-butanol had an antisenescence effects on the leaves of oat seedlings (Avena sativa). It both maintained chlorophyll levels and prevented proteolysis in the dark (Satler & Thimann 1980).
Maximum longterm immission concentration in air for plants, mg/m³	15 VDI 2306
Maximum longterm immission concentration in air for plants, ppm	5 VDI 2306

B

Effects on microorganisms	Toxicity data for microorganisms (WHO 1987):

Species	Conc.mg/l	Parameter	Reference
Protozoa			
Uronema parduczi (ciliate)	8	NOEC 20 hr total biomass	Bringmann& Kühn 1981
Chilomonas paramaecium (flagellate)	28	NOEC 48 hr total biomass	Bringmann & Kühn 1981
Entosiphon sulcatum (flagellate)	55	NOEC 72 hr total biomass	Bringmann & Kühn 1981
Bacteria			
Pseudomonas putida	650	NOEC 16 hr total biomass	Bringmann & Kühn 1981
Bacillus subtilis	1258	EC50 spore germination	Yasuda-Yasaki et al. 1978
	7400	no inhibition of, degradation by methane culture on acetate substrate	Chou et al.1978

Toxicity threshold (cell multiplication inhibition test):
Bacteria (Pseudomonas putida): 650 mg/l (Bringmann & Kühn 1980a)

EC50 values to microorganism, mg/l	2800	15 min Microtox (Hermens et al. 1985)
	10614	Biodegradation inhibition (Vaishnav 1986)
	3370	Microtox (Tarkpea et al. 1986)
EC50 values to algae, mg/l	8500	pht, Chlorella pyrenoidosa I (Jones 1971)
LOEC values to algae, mg/l	100	rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
NOEC values to algae, mg/l	875	8 d, grw, Scenedesmus quadricauda
	100	8 d, grw, Microcystis aeruginosa (Bringmann & Kühn 1978a)
LC50 values to crustaceans, mg/l	2100	96 hr, Nitocra spinipes (Linden et al. 1979)
EC50 values to crustaceans, mg/l	1880	24 hr, mbt, Daphnia magna (Bringmann & Kühn 1982)
	1900–2300	96 hr, Nitocra spinipes (Mattson et al.1976, Bentsson et al. 1984)
LC50 values to fishes, mg/l	1900–2300	24 hr, Semotitus atromaculatus (Gillette et al. 1952)
	1910	96 hr, rpd, Pimephales promelas (Vincent et al. 1976)
	1200	48 hr, Leucistus idus melanotus (Juhnke & Ludemann 1978)
	1900	24 hr, Carassius auratus (Bridie et al.1979a)
	1730–1910	96 hr, Pimephales promelas (Mattson et al.1976, Veith et al.1981,1983)
	2250–2400	96 hr, Alburnus alburnus (Linden et al. 1979, Bengtsson et al. 1984)

Other information about water organisms	At background concentrations likely to occur in the environment, 1-butanol is not directly toxic for fish, amphibia, or crustacea and is practically non toxic for algae. Some protozoa are slightly sensitive to 1-butanol (WHO 1987). Toxicity threshold (cell multiplication inhibition test): Algae (Microcystis aeruginosa): 100 mg/l (Bringmann & Kühn 1976) Green algae (Scenedesmus quadricauda): 875 mg/l Protozoa (Entosiphon sulcatum): 55 mg/l Protozoa (Uronema parduczi): 8.0 mg/l (Bringmann & Kühn 1980a) Algae (Chlorella pyrenoidosa: toxic: 8500 mg/l (Jones 1971).
Other effects on aquatic ecosystems	1-butanol should be managed in the environment as a slightly toxic compound. It poses an indirect hazard for the aquatic environment, because it is readily biodegradable, which may lead to oxygen depletion (WHO 1987).

352 • 2-Butanol

78-92-2

Synonyms	sec-Butyl alcohol secondary Butylalcohol Butylene hydrate 2-Hydroxy butane Methyl ethylcarbinol Butan-2-ol sec-Butanol SBA 2-Hydroxybutane CCS 301 2-Butylalcohol
Sumformula of the chemical	C4H10O
Use	The principal use of 2-butanol is as a chemical intermediate for conversion into methyl ethyl ketone, a solvent with a fairly high boiling point (Monich 1968). 2-butanol is used for the extraction of fish meal to produce fish protein concentrate. It is also used for the preparation of fruit essence and as a flavouring agent in food (Federal register 1977). Very recently, 2-butanol has proved to be useful as a debittering agent for protein hydrolysates (Latasidis & Sipberg 1978). 2-butanol is used, to some extent, as a solvent for lacquers, enamels, vegetable oils, gums, and natural resins; it is also used in hydraulic brake fluids, industrial cleaning compounds, polishes, and penetrating oils, and in the preparation of ore-flotation agents and perfumes (Patty 1963).
Restrictions to use	The Food Additives and Contaminants Committee (UK MAFF,1978) recommended that residues of butan-2-ol in food should not exceed 30 mg/kg (WHO 1987).
State and appearance	Colourless liquid.
Odour	Characteristic sweet odour. Hedonic tone: pleasant to neutral. Odour threshold: approximately 7.69 mg/m³ (2.5 ppm). (WHO 1987) Odour index (100% recognition): 28000 (Hellmann & Small 1974). Quality: sweet Hedonic tone: pleasant to neutral Threshold odour concentration: absolute: 0.12 ppm 50% recognition: 0.41 ppm 100% recognition: 0.56 ppm Odour index 100% recognition: 28 179 (Hellman & Small 1974).

Molecular weight	74.12	
Specific gravity (water=1)	0.808	at 20/4 °C
Vapour density (air=1)	2.55	
Density, kg/m³	806–808	
Conversion factor, 1 ppm in air=	3.078	mg/m³
Conversion factor, 1 mg/m³ in air=	0.325	ppm
Vapour pressure, mmHg	12 24	at 20 °C at 30 °C
Water solubility, mg/l	125000 201000 125000	at 20 °C at 30 °C (MITI 1992)
Melting point, °C	-89/-108 °C	
Boiling point, °C	99.5	(MITI 1992)
Log octanol/water coefficient, log Pow	0.65	(Sangster 1989)
Volatilization	Relative volatility (nBuAc=1) = 0.89	
Chemical oxygen demand, g 02/g	2.49	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	2.15	5 days (Bridie et al. 1979)
Total degradation in water	Biodegradation: 73.5% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
Other information about degradation	2-Butanol poses an indirect hazard for the aquatic environment, because it is readily biodegradable, which may lead to oxygen depletion (WHO 1987).	
Other information about bioaccumulation	2-butanol does not bioaccumulate (Chiou et al.1977).	
LD50 values to mammals in oral exposure, mg/kg	6500 4900 6480	orl-rat, US DHEW 1978 orl-rbt, Münch 1972 orl-rat (Patty 1967)
LD50 values to mammals in non-oral exposure, mg/kg	800	ipr-mus, US DHEW 1987
Effects on the reproduction of mammals	No relevant data on reproduction, embryotoxicity, or teratogenicity have yet been published (WHO 1987).	

Other information about mammals	In animals, 2-butanol is absorbed through lungs and gastrointestinal tract. No information is available regarding dermal adsorption. Approximately 97% of the dose of 2-butanol in animals is converted by alcohol dehydrogenase to the corresponding ketone, which is either excreted in the breath and urine of further metabolized (WHO 1987). The toxic effects from acute exposure are ataxia and narcosis. The potency of 2-butanol for intoxication is approximately 4 times that of ethanol. It is irritating to the eyes and non-irritating to the skin. From the animal studies available it is not possible to determine a NOEC level. No adequate data are available on mutagenicity, carcinogenicity, teratogenicity, or effects on reproduction (WHO 1987). Mouse: inhalation: no effect: 1650 ppm, 420 min (Patty 1967).
Health effects	In man the most likely acute effect of 2-butanol is alcoholic intoxication. No published data are available concerning other effects on man (WHO 1987).
Effects on plants	An EC50 of 650 mg/l was reported by Reynolds (1977) for seed germination in lettuce (Lactuca sativa). Inhibition of seed germination in cucumber (Cucumis sativus) was observed at 50375 mg 2-butanol/l (Smith & Siegel 1975).
Maximum longterm immission concentration in air for plants, mg/m³	15 VDI 2306
Maximum longterm immission concentration in air for plants, ppm	5 VDI 2306
Effects on microorganisms	Toxicity of 2-butanol for microorganisms (WHO 1987):

Species	*Conc. mg/l*	*Parameter*	*Reference*
Protozoa			
Uronema parduczi (ciliate)	1416	NOEC 20 hr total biomass	Bringmann & Kühn 1981
Chilomonas paramaecium (flagellate)	745	NOEC 48 hr total biomass	Bringmann & Kühn 1981
Entosiphon sulcatum (flagellate)	1282	NOEC 72 hr total biomass	Bringmann & Kühn 1981
Bacteria			
Pseudomonas putida	500	NOEC 16 hr total biomass	Bringmann & Kühn 1981
Bacillus subtilis	1630	EC50 spore germination	Yasuda-Yasaki et al. 1978

Toxicity threshold (cell multiplication inhibition test):
Bacteria (Pseudomonas putida): 500 mg/l (Bringmann & Kühn 1980a).

EC50 values to algae, mg/l	8900	pht, Chlorella pyrenoidosa (Jones 1971)
LOEC values to algae, mg/l	312	rpd, schr, Microcystis aeruginosa (Bringmann & Kuhn 1976)
	95	rpd, schr, Scenedesmus quadricauda (Bringmann & Kuhn 1980a)
NOEC values to algae, mg/l	95	8d, rpd, Scenedesmus quadricauda (Bringmann & Kuhn 1978a)
EC50 values to crustaceans, mg/l	2300	24 hr, mbt, Daphnia magna (Bringmann & Kuhn 1982)
LC50 values to fishes, mg/l	3520	48 hr, Leuciscus idus melanotus (Juhnke & Lüdeman 1978)
	4300	24 hr, Carassius auratus (Bridie et al. 1979)

Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): algae (Microcystis aeruginosa): 312 mg/l (Bringmann & Kühn 1976) green algae (Scenedesmus quadricauda): 95 mg/l protozoa (Entosiphon sulcatum): 1280 mg/l Protozoa (Uronema parduczi): 1416 mg/l (Bringmann & Kühn 1980a). Algae: Chlorella pyrenoidosa: toxic: 8900 mg/l (Jones 1971). Fish: goldfish: LD50 (24 hr): 4300 mg/l (Anon. 1975).

353 • tert-Butanol 75-65-0

Synonyms	2-Methyl-2-propanol tert Butyl alcohol tertiary Butanol Trimethyl carbinol TBA TMA t.Butyl hydroxide NCL-C55 Trimethyl methanol t-Butanol tert-Butylalcohol	
Sumformula of the chemical	C4H10O	
Use	The primary use of tert-butanol is as a solvent. It is also used as a dehydrating agent, in the extraction of drugs, in the manufacture of perfumes (particularly in the preparation of artificial musk), in the recrystallization of chemicals, and as a chemical intermediate (e.g., in the manufacture of tert-butyl chloride and in the manufacture of tert-butyl phenol). It is an approved denaturant for ethyl alcohol and for several other alcohols. Catalytic dehydration of tert-butanol is carried out to obtain isobutylene, and it has been patented for use as a gasoline antiknock agent. Moreover, it is used in the purification of polyolefins, for the separation of solids from coal liquids and as blowing agent for the manufacture of imide group-containing foams from copolymers of methacrylonitrile and methacrylic acid (Patty 1963, Monich 1968, Sherman 1978). As blending agent up to 7% to increase the octane rating of unleaded gasoline (Verschueren 1983).	
State and appearance	Solid (crystals).	
Odour	Camphor-like. Odour threshold approximately 144.7 mg/m³ (47 ppm).	
Molecular weight	74.12	
Specific gravity (water=1)	0.788	at 20/4 °C
Vapour density (air=1)	2.55	
Density, kg/m³	779–782	at 26 °C
Conversion factor, 1 ppm in air=	3.078	mg/m³
Conversion factor, 1 mg/m³ in air=	0.325	ppm
Vapour pressure, mmHg	31 42 56	at 20 °C at 25 °C at 30 °C
Melting point, °C	25.6	(MITI 1992)

Boiling point, °C	81.5 initial, min. 82.5 (MITI 1992)
Log octanol/water coefficient, log Pow	0.35 (Sangster 1989)
Chemical oxygen demand, g 02/g	2.49 5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.02 5 days (Bridie et al. 1979)
Total degradation in water	Biodegradation: 2.5% by BOD period: 28d substance: 100 mg/l sludge: 100 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Other information about degradation	In the short-term tests, there was little degradation but over a longer period of about one month, most of the material was fully degraded. Therefore, tert-butanol is inherently rather then readily biodegradable (WHO 1987).
Metabolism in mammals	In animals, tert-butanol is absorbed through the lungs and gastrointestinal tract; no information is available on dermal absorption. tert-butanol is not a substrate for alcohol dehydrogenase and is slowly metabolized by mammals. Up to 24% of the dose is eliminated in the urine as the glucoronide, and up to 10% of the dose can be excreted in the breath and urine as acetone or carbon dioxide (WHO 1987).
Bioconcentration factor, fishes	< 0.5 6w, Cyprinus carpio, conc 6 mg/l < 5 6w, Cyprinus carpio, conc 0.6 mg/l (MITI 1992)
Other information about bioaccumulation	tert-butanol does not bioaccumulate (Chiou et al. 1977). Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	3500 orl-rat (US DHEW 1979) 3600 orl-rbt (Münch 1972) 3500 orl-rat (Patty 1967)
LD50 values to mammals in non-oral exposure, mg/kg	1500 ivn-mus (Patty 1982) 900 ipr-mus (US DHEW 1978)
Effects on the reproduction of of mammals	No relevant data on reproduction, embryotoxicity, or teratogenicity have yet been published. In contrast to ethanol, tert-butanol at concentrations of 1000–4000 mg/l did not reduce the in vitro fertilizing capacity of mice spermatoa (Anderson et al. 1982, WHO 1987).
Other information about mammals	The primary acute effects observed in animals are signs of alcoholic intoxication. Its potency for intoxication is approximately 1.5 times that of ethanol. Animal data regarding skin and eye irritation are not available. tert-butanol produces physical dependence in animals and post-natal effects in offspring exposed in utero. Data on pathological effects of repeated exposure of animals are not available (WHO 1987).
Health effects	In man, tert-butanol is a mild irritant to the skin. There have not been any reports of poisonings or any other effects in man (WHO 1987).
Carcinogenicity	No adequate data are available on carcinogenicity, teratogenicity or effects on reproduction (WHO 1987).
Mutagenicity	Tert-butanol has been found not to be mutagenic (WHO 1987).
Effects on plants	An EC50 of 90800 mg/l was reported for germination in cucumber (Cucumis sativus) by Smith & Siegel (1975).

Effects on microorganisms	One study has indicated that Nitrosomonas (nitrifying bacterium) shows a high tolerance for tert-butanol; tert-butanol inhibits nitrifying activity at 39 400 mg/l (Blok 1981). There was no inhibition of degradation by methane culture on acetate substrate at 7400 mg tert-butanol /l (Chou et al. 1978).	
EC50 values to algae, mg/l	24200	Chlorella pyrenoidosa, pht (Jones 1971)
EC50 values to crustaceans, mg/l	7800	Artemia salina, excystment (Smith & Siegel 1975)
LC50 values to fishes, mg/l	3000–6000	24hr Semotitus atromaculutus (Gillette et al.1952)
	> 5000	24hr Carassius auratus (Bridie et al.1979)
	5500	48hr, Oryzias latipes (MITI 1992)
Other information about water organisms	Algae: Chlorella pyrenoidosa: toxic: 24200 mg/l (Jones 1971).	

354 • 2-Butanone

78-93-3

Synonyms	MEK Methylethylketone Methyl ethylketone Methyl acetone Butan-2-one	
Sumformula of the chemical	C4H8O	
Use	Solvent or swelling agent for resins, intermediate in the manufacture of ketones and amines, flush-off paint stripper, extraction and production of wax from lube oil fractions of petroleum, a solvent in nitrocellulose coatings and vinyl films.	
State and appearance	Colourless liquid.	
Odour	Quality: sweet, sharp Hedonic tone: neutral to unpleasant Threshold odour concentration absolute: 2.0 ppm 50% recognition: 5.5 ppm 100% recognition: 6.0 ppm Odour index 100% recognition: 15 350 (Hellman & Small 1974).	
Molecular weight	72.12	
Vapour pressure, mmHg	90.6	at 25 °C (Ambrose et al. 1975)
Water solubility, mg/l	268000 239000	20 °C (Valvani et al. 1981)
Melting point, °C	-86.3	
Boiling point, °C	79.6	
Log octanol/water coefficient, log Pow	0.3 0.29 0.29	Anon. 1986 (Hansch & Leo 1985) (Sangster 1989)
Henry's law constant, Pa x m³/mol	1.06	(Snider & Dawson 1985)
Volatilization	Relative volatility (nBuAc=1) = 3.70 The half-life for evaporation from a river and lake will be 3 and 12 days respectively. Due to its high vapour pressure, volatilation from soil will be rapid (Howard 1990).	

Mobility	Using the log Kow, a Koc value of 34 was estimated. Based on this estimated Koc value, MEK will be expected to exhibit very high mobility in soil and therefore may leach to the ground water (Lyman et al. 1982) (Swann et al. 1983).
Photochemical degradation in air	MEK adsorbs radiation near the sort wavelength cutoff of the solar spectrum at ground level; however the reaction with photochemically produced hydroxyl radicals with a half-life of 2.3 days is the dominant atmospheric process. Acetaldehyde is the primary product of this reaction (Cox et al. 1981).
Chemical oxygen demand, g 02/g	2.31 5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	2.03 5 days (Bridie et al. 1979)
Total degradation in soil	If 2-butanone is released to soil, it will partially evaporate into the atmosphere from near-surface soil and may leach into ground water. It will not significantly hydrolyze in soil (Howard 1990).
Total degradation in water	If 2-butanone is released into water, it will evaporate into the atmosphere with estimated half-lives of 3 and 12 days in rivers and lakes, respectively. It will also biodegrade slowly in both fresh and salt water. It may degrade slowly in anaerobic systems after a long acclimation period (Howard 1990).
Other information about degradation	Complete removal and 87% mineralization in 5 days in screening tests using municipal wastewater inocolum; complete removal in 9 days using activated sludge treatment (Dojlido 1979). Percent theoretical BOD in 5 and 20 days were 76% and 89%, respectively, using nonacclimated settled domestic wastewater inocolum in fresh water and 32% and 69%, respectively, using settled raw wastewater seed developed in actual seawater, with the test being run in synthetic seawater (Price et al. 1974). Percent theoretical BOD and COD were 76% and 79%, respectively, after 5 days at 20 °C using a standard dilution method with filtered biological sanitary waste treatment plant seed (Bridie et al. 1979). 88% theoretical BOD in 5 days using sew seed in standard dilution screening tests (Heukelekian & Rand 1955). Degradation also occurs in anaerobic systems but time required for acclimatising degrading microorganisms is long (ca 1 wk) (Chou et al. 1979).
Metabolism in mammals	Butan-2-one is readily absorbed by all routes of exposure; its metabolism appears to follow both oxidative and reductive pathways, the ketone undergoing omega-1 carbon atom oxidation to the corresponding hydroxyketone which then undergoes reduction to the diol. The secondary alcohol, butan-2-ole, is formed by the reduction of the ketone, and is then eliminated in the urine as O-sulfates and O-glucoronides, or may enter intermediary metabolism to be eliminated as carbon dioxide, or incorporated into tissues (Fawell & Hunt 1988, Williams 1959, Tadas et al. 1972, Munies 1965, DiVincenco et al. 1976, Wurster & Munies 1965, Tsao & Pfeiffer 1957, Zlatkis et al. 1973, Loney et al. 1963, Leibman 1971, Merritt & Tomkins 1959, Culp & McMahon 1968).
Other information about bioaccumulation	Using the log Kow a BCF of 1.0 was estimated. MEK will not be expected to significantly bioconcentrate in aquatic organisms (Howard 1990).
LD50 values to mammals in oral exposure, mg/kg	3400 orl-rat

B

Effects on the physiology of mammals	Few data are available concerning the long-term oral toxicity of butan-2-one. Short-term studies suggest that this ketone is of low oral toxicity. It also appears to have a low inhalation toxicity, and although it has been widely reported not to be neurotoxic itself, it does appear to potentiate polyneuropathy caused by other solvents. It is also thought that it may potentiate the hepatotoxicity of carbon tetrachloride, although it does not cause any hepatotoxic effects itself. These effects are believed to be due to induction of enzymes by the ketone (Carpenter 1954, Smyth et al. 1962, Kimura et al. 1971, Traiger & Bruckner 1975, Krasavage et al. 1982, US EPA 1976, Patty et al. 1935, Smyth 1956, La Belle & Brieger 1955, (Garcia et al. 1978), Abdel-Rahman et al. 1976, DiVincenzo & Krasavage 1974, NIOSH 1978, Moreno 1975, Carpenter 1949, Opdyke 1975, Spencer & Schaumberg 1976, Saida et al. 1975, Duckett et al. 1974, Shifman et al. 1981, Altenkirch et al. 1978, O'Donaghye et al. 1984, Hetland et al. 1976, Couri et al. 1977, Mellon Institute 1950, Clavender et al. 1983, Smith & Meyers 1944, Viader et al. 1975, Nakaaki 1974, Nelson et al. 1943, Elkins 1959, Malten et al. 1968, Rowe & Wolf 1963).
Effects on the reproduction of mammals	Reproductive toxicity studies have proved rather inconclusive, slight foetotoxic and embryotoxic effects being reported (Fawell & Hunt 1988, Schwetz et al. 1974, Deacon et al. 1981).
Mutagenicity	Butan-2-one was found to be non-mutagenic in Salmonella typhimurium TA98, TA100, TA1535, and TA1537, with and without S-9 from arcolor-induced Sprague-Dawley rats. The Ames tests were carried out at a concentration of 3 µmol/plate (Fawell & Hunt 1988, Florin et al. 1980).
Maximum longterm immission concentration in air for plants,mg/m³	30 VDI 2306
Maximum longterm immission concentration in air for plants,ppm	10 VDI 2306
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 1150 mg/l (Bringmann & Kühn 1980a)
EC50 values to microorganism, mg/l	20482 Biodegradation inhibition (Vaishnav 1986)
LOEC values to algae, mg/l	110 rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to crustaceans, mg/l	> 520 48 hr, Daphnia magna (LeBlanc 1980)
LC50 values to fishes, mg/l	1690 96 hr, Lepomis macrochirus (Turnbull et al. 1954) > 5000 24 hr, Carassius auratus (Bridie et al. 1979)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 4300 mg/l protozoa (Entosiphon sulcatum): 190 mg/l (Bringmann & Kühn 1980a)

355 • 2-Butanone oxime 96-29-7

Synonyms	Ethylmethylketoxime Methylethyl ketoxime
Sumformula of the chemical	CH3C(NOH)C2H5
Molecular weight	87.12
Specific gravity (water=1)	0.923 at 20/4 °C
Water solubility, mg/l	100000 > 12.5% MITI 1992
Melting point, °C	-29.5

B

Boiling point, °C	152	
Log octanol/water coefficient, log Pow	0.63	(MITI 1992)
Total degradation in water	Biodegradation: 24.7% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).	
Bioconcentration factor, fishes	0.5–0.6 < 2.5–5.8	6w, Cyprinus carpio, conc 2 mg/l 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
Effects on micro-organisms	Bacteria: Pseudomonas: still toxic at 630 mg/l (Meinck et al. 1970).	
LC50 values to fishes, mg/l	560	48 hr, Oryzias latipes (MITI 1992)
Other information about water organisms	Algae: Scenedesmus: still toxic at 1000 mg/l Protozoa: Colpoda: still toxic at 2500 mg/l (Meinck et al. 1970).	

356 • 1-Butene

106-98-9

Synonyms	Ethylethylene α-Butylene	
Sumformula of the chemical	CH3CH2CHCH2	
Odour	Characteristic; gashouse odour. Threshold Odour Concentration: 0.160 mg/m³ = 69 ppb (Stockham et al. 1969) Faint odour: 50–59 mg/m³ Odour Index: at 20 °C: 43480000 Threshold Odour Concentration: recognition: 39.2 mg/m³ 2.1 mg/m³ 1.2 mg/m³ (Verschueren 1983).	
Molecular weight	56.1	
Specific gravity (water=1)	0.67	liquefied
Vapour density (air=1)	1.94	
Conversion factor, 1 ppm in air=	1.23	mg/m³
Conversion factor, 1 mg/m³ in air=	430	ppm
Vapour pressure, mmHg	400 760	at - 21.7 °C at - 6.3 °C
Melting point, °C	-130	
Boiling point, °C	-6	
Henry's law constant, Pa x m3/mol	24800	calc. (Yaws et al. 1991)
Effects on plants	Tomato: epinasty in petiole: 50000 ppm, 2 days (Verschueren 1983).	

Other effects on aquatic ecosystems	Reduction of amenities: organoleptic limit: 0.2 mg/l (Verschueren 1983).

357 • cis-2-Butene 590-18-1

B

Sumformula of the chemical	CH3CH=CHCH3	
Odour	Odour thresholds: 4.8 mg/m³: recognition: 28.5 mg/m³ (Verschueren 1983).	
Molecular weight	56.1	
Specific gravity (water=1)	0.6	liquified
Vapour density (air=1)	1.94	
Conversion factor, 1 ppm in air=	2.33	mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.43	ppm
Boiling point, °C	4	
Log octanol/water coefficient, log Pow	2.33	(Sangster 1989)
Photochemical degradation in air	Estimated lifetime under photochemical smog conditions in S.E. England: 0.6 hr (Brice & Derwent 1978, Darnall et al. 1976).	

358 • trans-2-Butene 624-64-6

Synonyms	β-Butylene sym-Dimethylethylene	
Sumformula of the chemical	CH3CHCHCH3	
Odour	Odour threshold: recognition: 2700 mg/m³ (Verschueren 1983). Threshold odour concentration: 0.6 ppm Odour index: at 20 °C: 3333000 (Verschueren 1983).	
Molecular weight	56.1	
Specific gravity (water=1)	0.64	liquified
Vapour density (air=1)	1.94	
Conversion factor, 1 ppm in air=	2.33	mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.43	ppm
Vapour pressure, mmHg	760	at 0.9 °C
Melting point, °C	-105.4	
Boiling point, °C	1	
Log octanol/water coefficient, log Pow	2.31	(Sangster 1989)

359 • 3-Butenoic acid 625-38-7

Synonyms	Vinylacetic acid β-Butenoic acid

Sumformula of the chemical	CH2CHCH2COOH
Molecular weight	86.09
Specific gravity (water=1)	1.013 at 15/15 °C
Melting point, °C	-39
Boiling point, °C	163
Other information about water organisms	Algae: Chlorella pyrenoidosa: toxic: 280 mg/l (Jones 1971).

360 • 1-Butoxy-2-propanol 5131-66-8

Water solubility, mg/l	> 10000 (MITI 1992)
Total degradation in water	Biodegradation: 85–92% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

361 • Butoxycarboxim 34681-23-7

Use	Active ingredient in insecticides.
LC50 values to fishes, mg/l	1750 act, Cyprinus carpio (Pesticide Manual 1983)

362 • 2-Butoxyethanol 111-76-2

Synonyms	2-n-Butoxyethanol Butylcellosolve Butylglycolether Glycol monobutylether Butylglycol Ethyleneglycolmono-n-butylether
Sumformula of the chemical	C4H9OCH2CH2OH
Use	Solvent.
State and appearance	Colourless liquid.
Odour	Characteristic; sweet, ester. Hedonic tone: pleasant. Threshold Odour Concentration: absolute perception limit: 0.10 ppm 50% recognition: 0.35 ppm 100% recognition: 0.48 ppm Odour index: 100% recognition: 2729 (Hellmann & Small 1974). Odour index at 20 °C: 1650 (Verschueren 1983).
Molecular weight	118.17
Specific gravity (water=1)	0.903 at 20/4 °C
Vapour density (air=1)	4.07

Vapour pressure, mmHg	0.6	at 20 °C
Melting point, °C	< -40 °C	
Boiling point, °C	171–172	
Volatilization	Relative volatility (nBuAc=1) = 0.08	
Chemical oxygen demand, g 02/g	2.2	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.71	5 days (Bridie et al. 1979)
Total degradation in water	Biodegradation: 96.0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	2500 320 1200 1200 1480	orl-rat orl-rbt orl-mus orl-gpg (Patty 1967) -- orl-rat
Effects on the physiology of mammals	Rat: inhalation: 0/5, severely affected kidneys; 80 ppm, 4 hr (Patty 1967).	
Other information about mammals	Rat: inhalation: no effects; 20 ppm, 15 x 6 hr (Cage 1970). Rabbit: single oral dose; no effects: 0.5 ml/kg Rat: repeated oral dose: no effect: 0.125% in diet (Patty 1967).	
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 700 mg/l (Bringmann & Kühn 1980).	
LOEC values to algae, mg/l	35	rpd, schr, Microcystis aeruginosa (Bringmann & Kuhn 1976)
LC50 values to crustaceans, mg/l	800 775	48 hr, Crangon crangon 96 hr, Crangon crangon (Blackmann 1974)
LC50 values to fishes, mg/l	983 1490 1250 1700	7d, Poecilia reticulata (Könemann 1979) -- 96 hr, Lepomis macrochirus 96 hr, Menidia beryllina (Dawson et al.1977a) -- 24 hr, Carassius auratus (Bridie et al. 1979)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): algae (Microcystis aeruginosa): 35 mg/l (Bringmann & Kühn 1976) green algae (Scenedesmus quadricauda): 900 mg/l protozoa (Entosiphon sulcatum): 91 mg/l protozoa (Uronema parduczi): 463 mg/l (Bringmann & Kühn 1980).	

363 • Butyl acetoacetate 591-60-6

Synonyms	Acetoacetic n-butylester
Water solubility, mg/l	21000 (MITI 1992)
Total degradation in water	Biodegradtion: 82–86% by BOD period: 14d substance: 100mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

364 • sec-Butyl acetoacetate 13562-76-0

Synonyms	Acetoacetic sec-butylester
Water solubility, mg/l	18000 (MITI 1992)
Boiling point, °C	105–110, 40 mmHg (MITI 1992)
Total degradation in water	Biodegradation: 80–90% by BOD period: 21d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

365 • Butyl benzyl phthalate 85-68-7

Synonyms	BBP
Use	To plasticize or flexibilize synthetic resins, chiefly polyvinylchloride.
State and appearance	Clear oily liquid.
Molecular weight	312.39
Specific gravity (water=1)	1.1 at 25/25 °C
Vapour density (air=1)	10.8
Vapour pressure, mmHg	0.0000086 20 °C 1.9 200 °C
Water solubility, mg/l	2.9 –1.2
Melting point, °C	< -35 °C -40 (MITI 1992)
Boiling point, °C	370 (MITI 1992)
Log octanol/water coefficient, log Pow	4.78
Adsorption/desorption	Soil adsorption coefficient: 68–350 (Gledhill et al. 1980).

B

Total degradation in water	100% degradation in river water in 9 days (Verschueren 1983). 80% biodegradation in river water in 1 week (Johnson & Lulves 1975). Biodegradation: 81% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

Other information about degradation

	% degradation primary*	% degradation ultimate**	time days	half-life days
biodegradation				
activated sludge	93–99		1	
CO_2 evolution, aerobic		96	28	
gasproduction, anaerobic		< 10	28	
river water	100		9	2
lake water microcosm	> 95		7	< 4
lake water microcosm		51–65	28	
photodegradation	< 5		28	> 100
chemical degradation (hydrolysis)	< 5		28	> 100

*disappearance of BBP as measured by gas chromatography **mineralization under aerobic conditions to CO_2, under anaerobic conditions to H_2, CH_4 and CO_2 (Gledhill et al. 1980).

Bioconcentration factor, fishes	663	Lepomis macrochirus (Gledhill et al. 1980)
LD50 values to mammals in oral exposure, mg/kg	2330	orl-rat (Lewis & Sweet 1984)
LC50 values to mammals in inhalation exposure, mg/m³	13100	ihl-mam (Lewis & Sweet 1984)
Carcinogenicity	NTP carcinogenesis bioassay completed: results indefinite, rat; results negative, mus (Lewis & Sweet 1984).	
EC50 values to algae, mg/l	0.4 0.6	rpd, 96 hr, Selenastrum rpd, 96 hr, Skeletonema, Navicula (Gledhill et al. 1980)
NOEC values to algae, mg/l	0.1 0.1 0.3	rpd, schr, Selenastrum rpd, schr, Skeletonema rpd, schr, Navicula (Gledhill et al. 1980)
LC50 values to crustaceans, mg/l	92	48 hr, Daphnia magna (LeBlanc 1980)
EC50 values to crustaceans, mg/l	3.7	48 hr, Daphnia magna (Gledhill et al. 1980)
NOEC values to crustaceans, mg/l	1	srv, act, Daphnia magna (Gledhill et al. 1980)
LC50 values to fishes, mg/l	2.1–5.3 2.32 2.25 1.7 3.3	96 hr, Pimephales promelas 4 d, Pimephales promelas 14 d, Pimephales promelas 96 hr, Lepomis macrochirus 96 hr, Salmo gairdneri (Gledhill et al. 1980)

NOEC values to fishes, mg/l	0–2.2 srv, act, Pimephales promelas (Gledhill et al. 1980) 0.38 srv, act, Lepomis macrochirus (Gledhill et al. 1980) < 0.36 srv, act, Salmo gairdneri (Gledhill et al. 1980)

366 • tert-Butyl methacrylate 585-07-9

Synonyms	2-Methylpropenoic acid, tert-butyl ester
Sumformula of the chemical	C8H14O2
Water solubility, mg/l	50 (MITI 1992)
Boiling point, °C	67 70 mmHg (MITI 1992)
Log octanol/water coefficient, log Pow	2.54 (Sangster 1989)
Total degradation in water	Biodegradation: 32% by BOD (tert Butanol was remained) period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).

367 • p-t-Butyl-α-methylhydro cinnamic acid 66735-04-4

Sumformula of the chemical	C14H20O2
Melting point, °C	106–108 (MITI 1992)
Log octanol/water coefficient, log Pow	3.39 (MITI 1992)
Bioconcentration factor, fishes	< 0.1–0.6 6w, Cyprinus carpio, conc 0.1 mg/l < 0.9–15 6w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 20 48hr, Oryzias latipes (MITI 1992)

368 • 2-sec-Butyl-4,6-dinitrophenol 88-85-7

Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).

369 • 2-tert-Butyl-4,6-dinitrophenylacetate 3204-27-1

Synonyms	Dinoterpacetate
Use	Herbicide.
State and appearance	Pale yellow crystals.
Melting point, °C	133–134.5

B

LD50 values to mammals in oral exposure, mg/kg	> 4000 100 62 > 2000	orl-hens orl-rbt orl-rat orl-rat (Anon. 1976)
LC50 values to fishes, mg/l	0.068 0.039	24 hr, Rasbora heteromorpha 96 hr, Rasbora heteromorpha (Tooby et al. 1975)

370 • 2,6-tert-Butyl-4-cresol 128-37-0

Synonyms	2,6-Di-tert-butyl-p-cresol	
Sumformula of the chemical	C15H24O	
Melting point, °C	70	(MITI 1992)
Boiling point, °C	265	(MITI 1992)
Total degradation in water	Biodegradation: 4.5% by BOD period: 28d substance: 50 mg/l sludge: 50 mg/l (MITI 1992).	
Bioconcentration factor, fishes	230–2500 330–1800	8w, Cyprinus carpio, conc 0.05 mg/l 8w, Cyprinus carpio, conc 0.005 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be accumulated on a medium level (Anon. 1987).	
LC50 values to fishes, mg/l	5	48 hr, Oryzias latipes (MITI 1992)

371 • N-Butyl-N-ethyl-2,6-dinitro-4-trifluoromethylaniline 1861-40-1

Synonyms	Benefin Benfluralin Balan N-Butyl-N-ethyl-α,α,α-trifluoro-2,6-dinitro-p-toluidine Balane N-Butyl-2,6-dinitro-N-ethyl-4-trifluoromethylaniline N-Butyl-N-ethyl-2,6-dinitro-4-(trifluoromethyl)benzamine Quilan	
Sumformula of the chemical	C13H16F3N3O4	
Use	Herbicide.	
State and appearance	Yellow-orange crystals.	
Molecular weight	335.32	
Vapour pressure, mmHg	0.0000004 at 25 °C	
Melting point, °C	65–66.5 °C	
Log soil sorption coefficient, log Kom	4.03	(Sabljic 1987)

LD50 values to mammals in oral exposure, mg/kg	> 5000 > 2000 5 10	orl-mus orl-rbt, dog, ckn (Martin 1968) orl-mus) orl-rat (Sweet 1987
Other information about mammals	In diet; in 3 month feeding tests, the "safe" level for rats was 1250 ppm, for dogs 500 ppm (Martin 1968).	
Effects on plants	Benefin at 2 kg ai/ha gave complete control of crabgrass following nine consecutive annual applications (Callahan 1980). Weed groundcover of Ischaemum afrum was controlled by pre-planting herbicides in green-ridged groundnut: 1.68 kg benfluralin /ha was applied with a sprayer → a decrease in weed groundcover (Jenning & Drennan 1979).	
LC50 values to crustaceans, mg/l	1.1	96 hr, Gammarus fasciatus (Sanders 1970)
LC50 values to fishes, mg/l	1.2	96hr, Rasbora heteromorpha (Tooby et al. 1975)

372 • n-Butylacetate 123-86-4

Synonyms	Butylethanate Butylacetate Acetic acid butyl ester 1-Butyl acetate
Sumformula of the chemical	C6H12O2
Purity, %	90.92 CH3COOC4H9
Use	Solvents in production of lacquers, perfumes, natural gums and synthetic resins. Protective coatings.
State and appearance	Colourless liquid. Will float initially, dissolving at a fairly rapid rate.
Odour	Characteristic, sweet, ester, fruity. Hedonic tone: pleasant. Odour index (100% recognition): 284000 (Hellmann & Small 1974). Human odour perception: non perception: 0.5 mg/m³; perception: 0.6 mg/m³ Human reflex response: no response: 0.1 mg/m³; adverse response: 0.13 mg/m³ Animal chronic exposure: no effect: 0.1 mg/m³; adverse effect: 20 mg/m³ (Stern 1968). Distinct odour: 55 mg/m³ = 11 ppm (Verschueren 1983). Odour threshold in water: detection: 0.066 mg/kg (Flath et al.1967) 0.043 mg/kg (Sega et al. 1967). Quality: sweet, ester Hedonic tone: pleasant Threshold odour concetration absolute: 0.006 ppm 50% recognition: 0.037 ppm 100% recognition: 0.037 ppm Odour index 100% recognition: 284 300 (Hellman & Small 1974).

Molecular weight	116.16	
Specific gravity (water=1)	0.882	at 20/4 °C
Vapour density (air=1)	4	
Conversion factor, 1 ppm in air=	4.75	mg/m³
Conversion factor, 1 mg/m³ in air=	0.211	ppm
Vapour pressure, mmHg	10 15	at 20 °C at 25 °C
Water solubility, mg/l	14000 5000 7000	at 20 °C at 25 °C at 25 °C
Melting point, °C	-77.9 -76.8	
Boiling point, °C	126.5 117.5	
Flashing point, °C	29	
Log octanol/water coefficient, log Pow	1.82	(Sangster 1989)
Volatilization	Relative volatility (nBuAc=1) = 1.00	
Other physicochemical properties	Flammability: Moderate when exposed to heat or flame. Toxic combustion products: slightly hazardous. Explosiveness: Moderate – with flame. Reactive only under extreme conditions. Can react with oxidizing materials.	
Total degradation in water	0.1 mg/l affects the self purification of surface waters (Verschueren 1983).	
Other information about degradation	BOD, sewage, 5–20 days, 23.5–83% theo; Saltwater BOD, 5–20 days, 40–61% theo (Sax 1986). Will persist for several weeks (Sax 1986).	
LD50 values to mammals in oral exposure, mg/kg	4130 7060 14300 14000 7100 7400	orl-rat orl-mus 14d, orl-rat orl-rat orl-mus orl-rbt (Sax 1986)
LD50 values to mammals in non-oral exposure, mg/kg	> 17000 1230	14d, skn-rbt ipr-mus (Sax 1986)
LC50 values to mammals in inhalation exposure, ppm	2000	ihl-rat, 4 hr (Sax 1986)
LDLo values to mammals in non-oral exposure, mg/kg	1500	ipr-gpg (Sax 1986)
LCLo values to mammals in inhalation exposure, mg/kg	68000 67000	72 min, ihl-cat ihl-gpg, 4hr (Sax 1986)
Effects on the physiology of mammals	Guinea pig; eye irritation: 3300 ppm, 13 hr Cat: inhalation: some deaths: 17500 ppm, 30 min Cat: inhalation: loss of weight: 4200 ppm, 6 hr/day, 6 days (Patty 1967).	

Health effects	Man: mild eye and nose irritation: 200–300 ppm (Patty 1967). Man: unsatisfactory: > 200 ppm Symptoms of illness: 500 ppm Severe toxic effects: 2000 ppm, 60 min (Verschueren 1983). Narcotic. Skin irritation grade 1–no effects; may cause conjunctivitis. Eye irritation grade 5– burns from 0.005 ml (Sax 1986). Moderate ingestive and inhalative toxicant. Allergen (Sax 1986). Chronic hazard: Slight chronic toxicity hazard via all routes. Chronic allergen (Sax 1986). Skin and eye irritation data: eye, hmn, 300 ppm; skn, rbt, 500 mg, 24 hr, moderate; eye, rbt, 20 mg, severe (Sax 1986).
Maximum longterm immission concentration in air for plants,mg/m³	25 VDI 2306
Maximum longterm immission concentration in air for plants,ppm	5 VDI 2306
Effects on microorganisms	Bacteria: Escherichia coli: no toxic effect: 1 g/l. Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 115 mg/l (Bringmann & Kühn 1980).
LOEC values to algae, mg/l	280 rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976) 21 rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
LC50 values to crustaceans, mg/l	44 48 hr, Daphnia sp. (McKee & Wolf 1971)
LC50 values to fishes, mg/l	100 96 hr, Lepomis macrochirus 185 96 hr, Menidia beryllina (Dawson et al. 1977a) 62 96 hr, Branchydanio rerio 71–141 48 hr, Leuciscus idus (Wellens 1982)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): algae (Microcystis aeruginosa): 280 mg/l (Bringmann & Kühn 1976) green algae (Scenedesmus quadricauda): 21 mg/l protozoa (Entosiphon sulcatum): 321 mg/l protozoa (Uronema parduczi): 574 mg/l (Bringmann & Kühn 1980).

373 • tert-Butylacetate 540-88-5

Sumformula of the chemical	CH3COOC(CH3)3
State and appearance	Colourless liquid.
Specific gravity (water=1)	0.896 at 20 °C
Boiling point, °C	96
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 78 mg/l (Bringmann & Kühn 1980a).
LOEC values to algae, mg/l	420 rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)

Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): algae (Microcystis aeruginosa): 420 mg/l (Bringmann & Kühn 1976) green algae (Scenedesmus quadricauda): 3700 mg/l protozoa (Entosiphon sulcatum): 970 mg/l protozoa (Uronema parduczi): 1850 mg/l (Bringmann & Kühn 1980a).

374 • n-Butylacrylate 141-32-2

Synonyms	Propenoic acid, n-butyl ester	
Sumformula of the chemical	CH2CHCOOC4H9	
Use	Solvent.	
Molecular weight	128.2	
Specific gravity (water=1)	0.9	at 20/4 °C
Vapour density (air=1)	4.42	
Conversion factor, 1 ppm in air=	5.33	mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.19	ppm
Vapour pressure, mmHg	4 10	20 °C 36 °C
Water solubility, mg/l	1600	at 20 °C
Melting point, °C	-64	
Boiling point, °C	146.7	(MITI 1992)
Log octanol/water coefficient, log Pow	2.36	(Sangster 1989)
Volatilization	Relative volatility (nBuAc=1) = 0.42	
Total degradation in water	Biodegradation: 61% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	3700	orl-rat (Patty 1967)
LD50 values to birds in oral exposure, mg/kg	> 103	orl-Agelaius phoeniceus (Schafer et al. 1983)
Other information about water organisms	Threshold concentration of cell multiplication inhibition of the protozoa Uronema parduczi: 21 mg/l (Bringmann & Kühn 1980).	
Other effects on aquatic ecosystems	Reduction of amenities: organoleptic limit: 0.015 mg/l (Verschueren 1983).	

375 • Butylaldehyde 123-72-8

Synonyms	Butyraldehyde 1-Butanal Butyric aldehyde

Sumformula of the chemical	CH3CH2CH2CHO
Odour	Characteristic; sweet, rancid. Hedonic tone: unpleasant. Threshold Odour Concentration: absolute perception limit: < 0.0046 ppm 50% recognition: 0.0092 ppm 100% recognition: 0.039 ppm Odour Index: 2984615 (Hellmann & Small 1974). Threshold Odour Concentration: recognition: 0.013–0.014 mg/m³ 15 mg/m³ 0.042 mg/m³ (Verschueren 1983).
Molecular weight	72.1
Specific gravity (water=1)	0.817 at 20/4 °C
Vapour density (air=1)	2.48
Conversion factor, 1 ppm in air=	2.9 mg/m³
Conversion factor, 1 mg/m³ in air=	0.34 ppm
Vapour pressure, mmHg	71 20 °C
Water solubility, mg/l	200 (MITI 1992)
Melting point, °C	-99 (MITI 1992)
Boiling point, °C	75–76 °C 74.8 (MITI 1992)
Log octanol/water coefficient, log Pow	0.88 (Sangster 1989)
Total degradation in water	Biodegradation: 100% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	5900 orl-rat (Patty 1967)
LC50 values to mammals in inhalation exposure, ppm	60000 ihl-rat, 0.5 hr (Verschueren 1983)
Other information about mammals	Rat: inhalation: no effect: 1000 ppm, 12 x 6 hr (Cage 1970).
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 100 mg/l (Bringmann & Kühn 1980a).
LOEC values to algae, mg/l	19 rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to fishes, mg/l	25.8 96 hr, Pimephales promelas (Curtis & Ward 1981)

Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): algae (Microcystis aeruginosa): 19 mg/l (Bringmann & Kühn 1976) green algae (Scenedesmus quadricauda): 83 mg/l protozoa (Entosiphon sulcatum): 4.2 mg/l protozoa (Uronema parduczi): 98 mg/l (Bringmann & Kühn 1980a).
Other effects on aquatic ecosystems	Reduction of amenities: Threshold Odour Concentration: 0.009 mg/l Detection: 0.0373 mg/kg (Verschueren 1983).

376 • n-Butylamine 109-73-9

Synonyms	Norvalamine 1-Aminobutane Butylamine	
Sumformula of the chemical	$CH_3(CH_2)_3NH_2$	
Use	Intermediate for emulsifying agents; pharmaceuticals; insecticides; dyes; tanning agents.	
State and appearance	Colourless, volatile liquid.	
Odour	Characteristic, sour, ammoniacal. Hedonic tone: unpleasant to pleasant. Threshold Odour Concentration: absolute perception limit: 0.08 ppm 50% recognition: 0.24 ppm 100% recognition: 0.24 ppm Odour index: 100% recognition: 449166 (Hellmann & Small 1974). Odour index: at 20 °C: 395000 (Verschueren 1983).	
Molecular weight	73.1	
Specific gravity (water=1)	0.74	
Conversion factor, 1 ppm in air=	2.99	mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.334	ppm
Vapour pressure, mmHg	72	at 20 °C
Melting point, °C	-50	
Boiling point, °C	78	(MITI 1992)
Flashing point, °C	1.1	
pKa	10.64	(Sangster 1989)
Log octanol/water coefficient, log Pow	0.8 0.86	(Anon. 1986) (Sangster 1989)
Other physicochemical properties	Miscible with water, alcohol, ether.	

Total degradation in water	Biodegradation: 85% (NH_3) 66% (NO_2) by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
Effects on the physiology of mammals	Rat: inhalation: deaths: 4000 ppm, 4 hr Rat: inhalation: survived: 2000 ppm, 4 hr (Patty 1967).
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 800 mg/l (Bringmann & Kühn 1980).
Effects on wastewater treatment	Degradation by Aerobacter: 200 mg/l at 30 °C: parent: 100% in 22 hr mutant: 100% in 7 hr (Verschueren 1983).
LOEC values to algae, mg/l	0.14–0.19 rpd, schr Microcystis aeruginosa (Bringmann & Kuhn 1976) 0.53 rpd, schr, Scenedesmus quadricauda (Bringmann & Kuhn 1980a)
LC50 values to fishes, mg/l	32 96 hr, Lepomis macrochirus 24 96 hr, Menidia beryllina (Dawson et al. 1977a)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): algae (Microcystis aeruginosa): 0.14–0.19 mg/l (Bringmann & Kühn 1976) green algae (Scenedesmus quadricauda): 0.53 mg/l protozoa (Entosiphon sulcatum): 9 mg/l protozoa (Uronema parduczi): 1752 mg/l (Bringmann & Kühn 1980). Fish: Semolitus atromaculatus: critical range: 30–70 mg/l; 24 hr (McKee & Wolf 1963).

377 • sec-Butylamine 13952-84-6

Synonyms	2-Aminobutane 1-Methylpropyl amine 2-Butanamine	
Sumformula of the chemical	$C_4H_{11}N$	
Molecular weight	73.1	
Specific gravity (water=1)	0.72	
Vapour density (air=1)	2.52	
Conversion factor, 1 ppm in air=	2.99	mg/m³
Conversion factor, 1 mg/m³ in air=	0.334	ppm
Melting point, °C	–72	(MITI 1992)
Boiling point, °C	63	(MITI 1992)

Total degradation in water	Biodegradation: 68–109% by BOD (NH3) 53–94% by BOD (NO2) period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
Other information about degradation	Impact on biodegradation processes: at 100 mg/l no inhibition of NH3 oxidation by Nitrosomonas sp. (Verschueren 1983).
LD50 values to mammals in oral exposure, mg/kg	225 orl-dog 152 orl-rat (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	2500 skn-rbt (Sweet 1987)
Other information about mammals	Mammalia: rat: inhalation: discomfort, lethargy, retarded weight gain; autopsy: organs normal: 233 ppm, 13 x 6.5 hr (Verschueren 1983).
Other information about water organisms	Fish: creek chub: critical range: 20–60 mg/l; 24hr (Verschueren 1983).

378 • tert-Butylamine 75-64-9

Synonyms	2-Aminoisobutane 2-Amino-2-methylpropane 1,1-Dimethylethylamine Trimethylaminomethane Butylamine
Sumformula of the chemical	C4H11N
Use	Intermediate for rubber accelerators; insecticides; fungicides; dyestuffs; pharmaceuticals.
State and appearance	Colourless liquid slick, quickly dissolving.
Molecular weight	73.13
Specific gravity (water=1)	0.7
Vapour density (air=1)	2.5
Melting point, °C	-67.5
Boiling point, °C	44
Flashing point, °C	-8.85
pKa	10.68 (Sangster 1989)
Log octanol/water coefficient, log Pow	0.4 (Sangster 1989) Other physicochemical properties: Flammability: Quite. Flammable liquid. Toxic combustion products: heat decomposition emits toxic NOx fumes (Sax 1986). Explosiveness: Containers may rupture in a fire (Sax 1986). Very soluble in water (Sax 1986). Will form basic solution when dissolved in water (Sax 1986).
Other information about degradation	Nonpersistent (Sax 1986).

Other information about bioaccumulation	Not expected to accumulate in the food chain (Sax 1986).	
LD50 values to mammals in oral exposure, mg/kg	78 900 380	orl-rat orl-mus orl-rat (Sax 1986)
Health effects	Direct contact: Severe primary irritation and deep second-degree burns (blistering) in man; severe eye damage. General sensation: Fumes can cause burning and irritation of the eyes, nose, throat, and skin. Contact with the liquid can cause dermatitis and burns on the skin, lacrimation, conjunctivitis, corneal edema to the eyes. High vapour concentrations may cause nausea. Acute hazard level: tert-butylamine is very toxic to humans by ingestion; between 1 teaspoonful and 1 ounce may be fatal. Liquid can be absorbed through intact skin in harmful amounts (Sax 1986).	
Effects on wastewater treatment	Amenable to biological treatment at a municipal sewage treatment plant when diluted. Inhibits oxygen uptake (Sax 1986).	
EC50 values to algae, mg/l	16	rpd, 96hr, Selenastrum capricornutum (Calamari et al. 1982b)
LC50 values to crustaceans, mg/l	136	24hr, Daphnia magna (Calamari et al. 1982b)
LC50 values to fishes, mg/l	28 32 24	96hr, Salmo gairdneri (Calamari et al. 1980) 96hr, Lepomis macrochirus 96hr, silverside (Sax 1986)

379 • t-Butylamine borane 7337-45-3

Use	Fogging agent in photo processing.	
Molecular weight	86.97	
Degradation point, °C	98	
LC50 values to crustaceans, mg/l	0.7	Daphnia magna (Verschueren 1983)
LC50 values to fishes, mg/l	10 18	10–18, act, Pimephales promelas, (Verschueren 1983)
Other information about water organisms	Algae: Selenastrum capricornutum:	0.1 mg/l no effect 1.0 mg/l inhibitory (Anon. 1974).

380 • n-Butylbenzene 104-51-8

Synonyms	1-Phenylbutane	
Sumformula of the chemical	C10H14	
Use	Organic synthesis; pesticide manufacturing: solvent for coating compositions; plasticizer; surface active agents: polymer linking agent; asphalt component; naphtha constituent.	
Molecular weight	134.21	
Specific gravity (water=1)	0.86	at 20 °C
Vapour density (air=1)	4.62	
Vapour pressure, mmHg	1	at 23 °C
Melting point, °C	-81	

Boiling point, °C	183	
Log octanol/water coefficient, log Pow	4.26 4.13 4.26	(Anon. 1986) (Schwarzenbach & Westall 1981) (Sangster 1989)
Log soil sorption coefficient, log Kom	3.39 3.16	observed (Sabljic 1987) calculated (Sabljic 1987)
Other effects on aquatic ecosystems	Reduction of amenities: organoleptic limit: 0.1 mg/l (Verschueren 1983).	
Other information	Manufacturing source: petroleum refining.	

381 • sec-Butylbenzene 135-98-8

Synonyms	2-Phenylbutane	
Molecular weight	134.21	
Specific gravity (water=1)	0.862	at 20 °C
Vapour density (air=1)	4.62	
Vapour pressure, mmHg	1.1	at 20 °C
Melting point, °C	-83	
Boiling point, °C	173	

382 • tert-Butylbenzene 98-06-6

Synonyms	2-Methyl-2-phenylpropane	
Sumformula of the chemical	C10H14	
Molecular weight	134.21	
Specific gravity (water=1)	0.87	at 20 °C
Vapour density (air=1)	4.62	
Vapour pressure, mmHg	1.5	at 20 °C
Melting point, °C	-58	
Boiling point, °C	169	
Log octanol/water coefficient, log Pow	4.11	(Sangster 1989)
Other effects on aquatic ecosystems	Reduction of amenities: Threshold Odour Concentration: 0.05 mg/l (Zoeteman et al. 1971).	

383 • p-tert-Butylbenzoic acid 98-73-7

Synonyms	PTBBA p-tert-Butyl benzoic acid	
State and appearance	Colourless crystalline powder.	
Specific gravity (water=1)	1.142	at 20/4 °C
Water solubility, mg/l	28	(MITI 1992)
Melting point, °C	166.9	(MITI 1992)

Log octanol/water coefficient, log Pow	1.98	(MITI 1992)
Chemical oxygen demand, g 02/g	2.37	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.26	5 days (Bridie et al. 1979)
Total degradation in water	Biodegradation: 0–12% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	1.1–2.0 < 4.6	6w, Cyprinus carpio, conc 0.5 mg/l 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
LD50 values to mammals in oral exposure, mg/kg	735 568	orl-rat orl-mus (Anon. 1975)
LC50 values to fishes, mg/l	4 33 92	pH 5, 96 hr, Carassius auratus pH 7, 96 hr, C.auratus (Anon.1975) 48hr, Oryzias latipes (MITI 1992)

384 • Butylbutyrate

109-21-7

LC50 values to fishes, mg/l	11.6	96hr, Pimephales promelas (Curtis & Ward 1981)

385 • Butylcarbitolacetate

124-17-4

Synonyms	Butyldigolacetate	
Sumformula of the chemical	C4H9OCH2CH2OCH2CH2OOCCH3	
Specific gravity (water=1)	0.98	at 20 °C
Vapour density (air=1)	7.02	
Vapour pressure, mmHg	0.04	at 20 °C
Water solubility, mg/l	65000 31100	at 20 °C (MITI 1992)
Melting point, °C	< -10	(MITI 1992)
Boiling point, °C	247.7–249.4 (MITI 1992)	
Total degradation in water	Biodegradation: 100–102% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

386 • p-tert-Butylcatechol

98-29-3

Synonyms	4-tert-Butylpyrocatechol 4-tert-Butyl-1,2-dihydroxybenzene

Use	Polymerization inhibitor for styrene-butadiene and other olefins.
State and appearance	White crystalline solid.
Odour	In water: odour threshold: detection: 1.0 mg/l (Verschueren 1983).
Molecular weight	166.22
Specific gravity (water=1)	1.05 at 60/25 °C
Vapour pressure, mmHg	0.0028 at 25 °C
Melting point, °C	56–58
Boiling point, °C	285
LD50 values to mammals in oral exposure, mg/kg	2820 orl-rat 200–800 orl-gpg (Verschueren 1983)
LD50 values to birds in oral exposure, mg/kg	> 96 orl-Agelaius phoeniceus (Schafer et al. 1983)

387 • Butylcellosolveacetate 112-07-2

Synonyms	Ethyleneglycol monobutyl ether acetate
Sumformula of the chemical	C4H9OCH2CH2OOCCH3
Use	High boiling solvent for nitrocellulose lacquers, epoxy resins.
State and appearance	Colourless liquid.
Odour	Quality: sweet, ester Hedonic tone: pleasant. Threshold Odour Concentration: absolute perception limit: 0.11 ppm 50% recognition: 0.20 ppm 100% recognition: 0.20 ppm Odour index 100% recognition: 6 550 (Hellman & Small 1974).
Specific gravity (water=1)	0.94 at 20/20 °C.
Boiling point, °C	192.3

388 • n-Butylchloride 109-69-3

Synonyms	1-Chlorobutane
Sumformula of the chemical	CH3(CH2)2CH2Cl
Odour	Characteristic; pungent. Hedonic tone: unpleasant. Threshold Odour Concentration: absolute perception limit: 8.82 ppm 50% recognition: 13.3 ppm 100% recognition: 16.7 ppm Odour Index: 6377 (Hellmann & Small 1974).
Molecular weight	92.57
Specific gravity (water=1)	0.884
Vapour density (air=1)	3.2

Vapour pressure, mmHg	80.1	at 20 °C
Water solubility, mg/l	660 370	at 12 °C (MITI 1992)
Melting point, °C	-123.1	(MITI 1992)
Boiling point, °C	78.5	(MITI 1992)
Log octanol/water coefficient, log Pow	2.64 2.82	(Sangster 1989) (MITI 1992)
Henry's law constant, Pa x m³/mol	1708	calc. (Yaws et al. 1991)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 5.21 mg/l sludge: 2 mg/l (MITI 1992).	
Bioconcentration factor, fishes	7.6–21 11–17	6w, Cyprinus carpio, conc 0.5 mg/l 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
LC50 values to fishes, mg/l	97 79.9	7 d, Poecilia reticulata (Könemann 1979) 48hr, Oryzias latipes (MITI 1992)

389 • 1,2-Butyleneoxide

106-88-7

Odour	Characteristic; sweet, alcohol. Hedonic tone: pleasant. Threshold Odour Concentration: absolute perception limit: 0.07 ppm 50% recognition: 0.71 ppm 100% recognition: 0.71 ppm Odour Index: 260563 (Hellmann & Small 1974).	
Molecular weight	72.1	
Specific gravity (water=1)	0.83	
Vapour density (air=1)	2.49	
Conversion factor, 1 ppm in air=	2.94	mg/m³
Conversion factor, 1 mg/m³ in air=	0.34	ppm
Water solubility, mg/l	82400	at 25 °C
Melting point, °C	-60	
Boiling point, °C	65	
LD50 values to mammals in oral exposure, mg/kg	500	orl-rat (Verschueren 1983)
Other information about mammals	Rat, guinea pigs, rabbits: inhalation; repeated 7 hr exposures at 400 ppm can be tolerated for prolonged periods (Patty 1967).	

B

390 • n-Butylether

142-96-1

Synonyms	Di-n-Butylether 1-Butoxybutane	
Sumformula of the chemical	C4H9OC4H9	
Use	Solvent for hydrocarbons; fatty materials; extracting agent.	
Odour	Characteristic: fruity, sweet. Hedonic tone: pleasant. Threshold Odour Concentration: absolute perception limit: 0.07 ppm 50% recognition: 0.24 ppm 100% recognition: 0.47 ppm Odour Index: 13978 (Hellmann & Small 1974). Detection: 8 mg/m³ (Verschueren 1983).	
Molecular weight	130.2	
Specific gravity (water=1)	0.769	at 20/20 °C
Vapour density (air=1)	4.5	
Conversion factor, 1 ppm in air=	5.33	mg/m³
Conversion factor, 1 mg/m³ in air=	0.188	ppm
Vapour pressure, mmHg	4.8	
Water solubility, mg/l	300 330	at 20 °C (MITI 1992)
Melting point, °C	-95	
Boiling point, °C	141	
Log octanol/water coefficient, log Pow	3.21 3.35	(Sangster 1989) (MITI 1992)
Total degradation in water	Biodegradation: 3–4% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	47–83 30–114	6w, Cyprinus carpio, conc 0.2 mg/l 6w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987) (dibutyl ether).	
LD50 values to mammals in oral exposure, mg/kg	7400	orl-rat (Patty 1967)
Health effects	Man: irritation of eyes and nose: 200 ppm (Patty 1967).	
LC50 values to crustaceans, mg/l	26	48 hr, Daphnia magna (LeBlanc 1980)
LC50 values to fishes, mg/l	30.7	48hr, Oryzias latipes (MITI 1992)
Other information about water organisms	Threshold concentration of cell multiplication inhibition of the protozoa Uronema parduczi: > 40 mg/l (Bringmann & Kühn 1980).	

391 • n-Butylformate

592-84-7

Sumformula of the chemical	HCOOC4H9
Odour	Detection: 6.0 mg/kg Threshold Odour Concentration: 17 ppm = 70 mg/m³ distinct odour: 60 mg/m³ = 20 ppm (Verschueren 1983).
Molecular weight	102.13
Specific gravity (water=1)	0.8885 at 20/4 °C
Vapour density (air=1)	3.5
Conversion factor, 1 ppm in air=	4.17 mg/m³
Conversion factor, 1 mg/m³ in air=	0.24 ppm
Vapour pressure, mmHg	30 at 25 °C
Melting point, °C	-90
Boiling point, °C	106.8
Other information about mammals	Cat: inhalation: death: 10000 ppm, 60 min Dog: inhalation: narcosis: 10000 ppm, 60 min (Patty 1967).
Health effects	Man: intolerable irritation: 10000 ppm, < 1 min (Patty 1967).
Other effects on aquatic ecosystems	Reduction of amenities: Threshold Odour Concentration: 6.0 mg/l (Verschueren 1983).

392 • Butylglycidylether

2426-08-6

Synonyms	n-Butylglycidylether BGE 1-Butoxy-2,3-epoxypropane 3-Butoxy-1,2-epoxypropane 2,3-Epoxypropylbutylether Butyl-2,3-epoxypropylether Glycidylbutylether (Butoxymethyl)oxirane
Use	Component of epoxy resin systems. The epoxy group of the glycidylether reacts during the curing process and glycidylethers are therefore generally no longer present in completely cured products.
State and appearance	Colourless liquid.
Odour	Characteristic. Hedonic tone: irritating, not unpleasant.
Molecular weight	130.21
Specific gravity (water=1)	0.908 at 25/4 °C
Conversion factor, 1 ppm in air=	5.32 mg/m³
Conversion factor, 1 mg/m³ in air=	0.188 ppm
Vapour pressure, mmHg	3.2 at 25 °C
Water solubility, mg/l	20000 at 20 °C

Boiling point, °C	164–168
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
LD50 values to mammals in non-oral exposure, mg/kg	1530 intragastric-mus 2260 intragastric-rat (Patty 1967)
Effects on the physiology of mammals	Rat: inhalation: retarded growth: 150 ppm, 50 x 7 hr (Patty 1967). Rat: inhalation: 7 hr/d, 5 d/w, 50 exposures: 75 ppm: slight patchy atrophy of the testes in 1 of 10 animals; 300 ppm: atrophic testes in 5 of 10 animals (Verschueren 1983).
Other information about mammals	Rat: inhalation: no signs of toxicity: 75 ppm, 50 x 7 hr rat: inhalation: chronic toxicity: 300 ppm, 50 x 7 hr (Patty 1967).

393 • n-Butylmercaptan 109-79-5

Synonyms	Butanethiol
Sumformula of the chemical	C4H9SH
Odour	Characteristic, strong, unpleasant. Odour Index at 20 °C: 49000000 (Verschueren 1983).
Molecular weight	90.18
Specific gravity (water=1)	0.84 at 20 °C
Vapour density (air=1)	3.1
Conversion factor, 1 ppm in air=	3.75 mg/m³
Conversion factor, 1 mg/m³ in air=	0.27 ppm
Water solubility, mg/l	590 at 22 °C
Melting point, °C	-116
Boiling point, °C	98
Log octanol/water coefficient, log Pow	2.28 (Sangster 1989)
LC50 values to fishes, mg/l	1100 4d, Ictalurus punctatus 3600 4d, Ictalurus punctatus (Mather-Mihaich & Di Giulio 1986)
Effects on the physiology of water organisms	Ictalurus punctatus: 500 mg/l, 21 days; enzyme effect (change in enzyme activity) 80 mg/l, 21 days; haematological effect (change in various blood parameters such as red blood cell count, haematocrit, and serum osmolarity) (Mather-Mihaich & Di Giulio 1986).
Other effects on aquatic ecosystems	Reduction of amenities: Threshold Odour Concentration: average: 0.006 mg/l range: 0.001 to 0.06 mg/l (Verschueren 1983).

394 • p-tert-Butylphenol

98-54-4

Synonyms	4-(α,α-Dimethylethyl)phenol 4-tert-Butylphenol 4-(1,1-Dimethylethyl)phenol Butylphen 1-Hydroxy-4-tert-butylbenzene
Sumformula of the chemical	C10H14O
State and appearance	White aromatic flake.
Molecular weight	150.21
Specific gravity (water=1)	0.908 at 114/4 °C
Water solubility, mg/l	700
Melting point, °C	98–98.5 (MITI 1992)
Boiling point, °C	236.5 (MITI 1992)
Log octanol/water coefficient, log Pow	3.04 (Sangster 1989)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Other information about degradation	Impact on biodegradation processes: inhibition of degradation of glucose by Pseudomonas fluorescents at: 25 mg/l; inhibition of degradation of glucose by Escherichia coli at: > 100 mg/l (Bringmann & Kühn 1960).
Bioconcentration factor, fishes	20–43 8w, Cyprinus carpio, conc 0.04 mg/l < 48–88 8w, Cyprinus carpio, conc 0.004 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	400–2000 orl-gpg (Verschueren 1983) 1500 orl-mam 2951 orl-rat (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	78 ipr-mus 1580 skn-mam 2288 skn-rbt (Sweet 1987)
TDLo values to mammals in oral exposure, mg/kg	252 orl-ham, tumorigenic (Sweet 1987)
Effects on microorganisms	Bacteria: Escherichia coli: LD0: > 100 mg/l (Meinck et al. 1970).
LC50 values to fishes, mg/l	5.14 96 hr, Pimephales promelas (Holcombe et al. 1984) 0.74 96 hr, juv., Salmo salar (McLeese et al. 1981) 4 48 hr, Oryzias latipes (MITI 1992)

Other information about water organisms	Algae: Scenedesmus: LD0: 10 mg/l Arthropoda: Daphnia: LD0: 8 mg/l (Meinck et al. 1970).
Other effects on aquatic ecosystems	Reduction of amenities: odour threshold: detection; 0.8 mg/l; approximate concentration causing adverse taste in fish: 0.03 mg/l (Verschueren 1983).

395 • p-sec-Butylphenyl-2,3-epoxypropylether 67557-76-0

Sumformula of the chemical	C13H18O2
Log octanol/water coefficient, log Pow	2.71 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD (hydrolyzed to p-sec-Butylphenyl-2,3-dihydroxypropylether) period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).

396 • o-sec-Butylphenyl-N-methylcarbamate 3766-81-2

Synonyms	BPMC
Use	BPMC is one of several carbamate insecticides applied in large quantities in Japan to control plant hoppers and leafhoppers on rice plants.
Water solubility, mg/l	680 (MITI 1992)
Melting point, °C	26.5–31 (MITI 1992)
Boiling point, °C	112–113, 0.2 mmHg (MITI 1992)
Log octanol/water coefficient, log Pow	2.79 (MITI 1992)
Total degradation in soil	Disappearance in Saga soil at 30 °C humidity: at 0.2 ppm initial concentration 55% BPMC remained in paddy soil after 50 days; at 1.0 ppm initial concentration 45% BPMC remained in paddy soil after 50 days; at 10 ppm initial concentration 5% BPMC remained in paddy soil after 50 days; since the disappearance rate of BPMC in soils was retarded by addition of sodium azide, it was suggested that soil microorganisms participated in the degradation of BPMC (Masako & Kanazava 1979).
Total degradation in water	Biodegradation: 0–1% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.2–3.3 6w, Cyprinus carpio, conc 0.02 mg/l < 1.9–4.0 6w, Cyprinus carpio, conc 0.002 mg/l (MITI 1992)
LC50 values to fishes, mg/l	9.93 48hr, Oryzias latipes (MITI 1992)

397 • n-Butylphosphoric acid

12788-93-1

Synonyms	Acid butylphosphate
Use	Esterification catalyst and polymerizing agent ; curing catalyst and accelerator in resins and coatings; special detergents.
State and appearance	Water white liquid.
Specific gravity (water=1)	1.120–1.125 at 25/4 °C
Flashing point, °C	110
Log octanol/water coefficient, log Pow	0.28
Other physicochemical properties	Soluble in alcohol, acetone, and toluene. Insoluble in water and petroleum naphtha. Combustible.
Health effects	Strong irritant to skin & tissue.
Effects on microorganisms	Bacteria: Pseudomonas putida: inhibition of cell multiplication starts at > 100 mg/l (Bringmann & Kühn 1976).
Other information about water organisms	Algae: Microcystis aeruginosa: inhibition of cell multiplication starts at 4.1 mg/l (Bringmann & Kühn 1976).

398 • n-Butylsulfide

544-40-1

Synonyms	Dibutylsulfide Butylthiobutane	
Sumformula of the chemical	CH3CH2CH2CH2)2S	
Odour	Hedonic tone: unpleasant. Threshold Odour Concentration: 0.012 mg/m³ = 2 ppb (Stockham et al. 1969). Odour Index: at 20 °C: 658000 (Verschueren 1983).	
Molecular weight	146.29	
Specific gravity (water=1)	0.839	at 16/0 °C
Vapour pressure, mmHg	1 10 40	at 21.7 °C at 66.4 °C at 96.0 °C
Melting point, °C	-79.7	
Boiling point, °C	182	
Other effects on aquatic ecosystems	Reduction of amenities: faint odour: at 0.0011 mg/l (Verschueren 1983).	

399 • p-tert-Butyltoluene

98-51-1

Synonyms	1-Methyl-4-tert-butylbenzene 8-Methylparacymene PTBT	
Odour	Immediate recognition at 5 ppm (Patty 1967).	
Molecular weight	148.25	
Specific gravity (water=1)	0.857	at 20/20 °C
Conversion factor, 1 ppm in air=	6.05	mg/m³

Conversion factor, 1 mg/m³ in air=	0.16	ppm
Water solubility, mg/l	< 10	(MITI 1992)
Melting point, °C	-62.53	
Boiling point, °C	189–192	(MITI 1992)
Log octanol/water coefficient, log Pow	5.17	(MITI 1992)
Chemical oxygen demand, g 02/g	2.56	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.06	5 days (Bridie et al. 1979)
Total degradation in water	Biodegradation: 30–65% by BOD (Trimethyl acetic acid was remained) period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
LC50 values to mammals in inhalation exposure, ppm	165 248 934	ihl-rat, 8 hr) ihl-rat, 4 hr ihl-rat, 1 hr (Patty 1967
Other information about mammals	Rat: inhalation: LC50: no unusual behaviour: 50 ppm, 7 hr/day, 25 days (Patty 1967). Rabbit: percutane LD50: 13.8–27.8 ml/kg (Patty 1967).	
Health effects	Man: moderate eye irritation: 80 ppm, 5 min (Patty 1967).	
LC50 values to fishes, mg/l	3	24hr, Carassius auratus (Anon. 1975)

400 • 2-Butyne-1,4-diol 110-65-6

Synonyms	1,4-Butynediol 2-Butynediol	
LD50 values to birds in oral exposure, mg/kg	75 > 75.0	orl-Agelaius phoeniceus orl-Coturnix coturnix (Schafer et al. 1983)

401 • Butyramide 541-35-5

Synonyms	Butanamide Butyric amide	
Sumformula of the chemical	CH3CH2CH2CONH2	
Molecular weight	87.12	
Specific gravity (water=1)	1.032	at 20/4 °C
Water solubility, mg/l	162800	at 15 °C
Melting point, °C	116	
Boiling point, °C	216	
Log octanol/water coefficient, log Pow	-0.21	(Sangster 1989)

LD50 values to birds in oral exposure, mg/kg	> 96	orl-Agelaius phoeniceus (Schafer et al. 1983)

402 • Butyranilide

1129-50-6

Sumformula of the chemical	C10H13NO	
Log soil sorption coefficient, log Kom	1.47	(Sabljic 1987)

403 • n-Butyric acid

107-92-6

Synonyms	n-Butanoic acid Ethylacetic acid	
Sumformula of the chemical	CH3(CH2)2COOH	
State and appearance	Colourless liquid.	
Odour	Sour.	
Molecular weight	88.1	
Specific gravity (water=1)	0.959	at 20/4 °C
Vapour density (air=1)	3.04	
Conversion factor, 1 ppm in air=	3.66	mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.27	ppm
Vapour pressure, mmHg	0.43 1.4	at 20 °C at 30 °C
Water solubility, mg/l	56200	at - 1.1 °C
Melting point, °C	- 5.5/- 8 °C	
Boiling point, °C	163.7	at 757 mm
pKa	4.82	
Log octanol/water coefficient, log Pow	0.79	(Sangster 1989)
LD50 values to mammals in oral exposure, mg/kg	2900–3800	orl-rat (Patty 1967)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 875 mg/l (Bringmann & Kühn 1980).	
LOEC values to algae, mg/l	318	rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to crustaceans, mg/l	61	48hr, Daphnia magna (Dowden & Bennett 1965)

Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): algae (Microcystis aeruginosa): 318 mg/l (Bringmann & Kühn 1976) green algae (Scenedesmus quadricauda): 2600 mg/l protozoa (Entosiphon sulcatum): 26 mg/l protozoa (Uronema parduczi): 129 mg/l (Bringmann & Kühn 1980). Algae: Chlorella pyrenoidosa: toxic: 340 mg/l (Jones 1971). Scenedesmus: toxic: 200 mg/l (Meinck et al. 1970). Protozoa: Vorticella campanula: toxic: 10 mg/l (Meinck et al. 1970) Paramaecium caudatum: toxic: 250 mg/l Arthropoda: Daphnia: toxic: 60 mg/l (Meinck et al. 1970) Mollusca: Limnea ovata: toxic: 50 mg/l

404 • γ-Butyrolactone 96-48-0

Sumformula of the chemical	C4H602
EINECS-number	2025095
Water solubility, mg/l	> 100000(MITI 1992)
Melting point, °C	-43.53 (MITI 1992)
Boiling point, °C	204 (MITI 1992)
Total degradation in water	Biodegradation: 62–90% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

405 • Butyronitrile 109-74-0

Synonyms	Butanenitrile n-Propylcyanide Cyanopropane
Sumformula of the chemical	CH3CH2CH2CN
State and appearance	Colourless liquid.
Molecular weight	69.1
Specific gravity (water=1)	0.8 at 20 °C
Vapour density (air=1)	2.4
Vapour pressure, mmHg	10 at 15 °C 40 at 38 °C
Melting point, °C	-112.6
Boiling point, °C	118
Log octanol/water coefficient, log Pow	0.6 (Sangster 1989)
Other information about degradation	Biodegradation by a mutant microorganism: 500 mg/l at 20 °C: parent: 100% disruption in 13 hr mutant: 100% disruption in 4 hr (Verschueren 1983).

LD50 values to mammals in oral exposure, mg/kg	50–100 orl-rat (Patty 1967)
Effects on the physiology of mammals	Rat: inhalation: no toxic signs, daily urinary thiocyanate: 0.006 mg (normal 0.00007 mg): autopsy: organs normal: 200 ppm, 20 x 6 hr (Cage 1970).

406 • Cacodylic acid

75-60-5

Synonyms	Hydroxydimethylarsine oxide Dimethylarsinic acid
Sumformula of the chemical	(CH3)2AsO2H
Products containing the chemical	Phytar Ansar Phytar 138 * 65.6% cacodylic acid
Use	Contact herbicide; cotton defoliant; nonselective contact herbicide on noncrop areas.
State and appearance	Colourless crystals.
Odour	Odourless.
Water solubility, mg/l	2000000 at 25 °C
Melting point, °C	192–198 °C
Aerobic degradation in soil	The degradation of cacodylic acid in soils proceeds by two mechanisms. Under aerobic conditions 35% was converted to a volatile organoarsenical compound and 41% to CO2 and AsO4-3 within a 24-week period (Woolson & Kearney 1973).
Anaerobic degradation in soil	The degradation of cacodylic acid in soils proceeds by two mechanisms. Under anaerobic conditions 61% was converted to a volatile organoarsenical within a 24-week period and was lost from soil system. The ultimate environmental fate of the arsenic from cacodylic acid appears to be metabolized to inorganic arsenate which is bound as insoluble compounds in the soil (Woolson & Kearney 1973).
LD50 values to mammals in oral exposure, mg/kg	1350 technical product, orl-rat (Martin 1968)
LD50 values to mammals in non-oral exposure, mg/kg	720 ipr-rat, male 520 ipr-rat, female 520 ipr-mus, male 600 ipr-mus, female (Martin 1968)

407 • Cadmium and cadmium compounds

7440-43-9

Sumformula of the chemical	Cd
Use	Electrodeposited and dipped coatings on metals, bearing and low-melting alloys, brazing alloys, fire protection systems, nickel-cadmium storage batteries, power transmission wire, TV phosphors, basis on pigments used in ceramic glazes, machinery enamels, baking enamels, Weston standard cell control of atomic fission in nuclear reactors, fungicide, photography an lithography, selenium rectifiers, electrodes for cadmium-vapour lamps and photoelectric cells.
State and appearance	Soft, blue-white, malleable metal or grayish-white powder.
Molecular weight	112.4
Melting point, °C	320.9
Boiling point, °C	767

C

Adsorption/desorption	Adsorption by clay minerals and to a less degree by iron- and manganese oxides seem to be the most important immobilizing processes in soil (Farrah & Pickering 1977).	
Mobility	The mobility of Cd in soils is controlled mainly by pH and redox potential (Farrah & Pickering 1977). In fresh waters Cd usually is in ion form (Cd2+). The mobility of Cd i controlled mainly by pH and organic material. In brackish waters and in marine environment Cd appears usually as chloride complexes CdCl+ and CdCl2 (Zirino & Yamamoto 1972). Soluble in acids, especially nitric, and in ammonium nitrate solution. Combustible. Flammable in powder form (Sax & Lewis 1987).	
Metabolism in mammals	The metabolism of cadmium in animals is characterized by the absence of effective homeostatic mechanisms and retention which results in long biological half-lives: rat: 200 days; mouse: 25–100 days; dog: 260–500 days (Nyholm 1985). Interactions between Cd and essential bivalent metals (Zn, Cu, Fe, Ca) is very important in absorption and metabolism (Nyholm 1985).	
Metabolism in fishes	Cd is accumulated mainly in kidneys, gills and alimentary canal of fish. No correlation between Cd concentration in fish musclular system and Cd concentration in water (Bengtsson 1980c). Cd concentration in fish exposed to Cd in fresh water for 10 and 24 days was 6–10 times higher as Cd concentration in fish exposed to Cd in brackish water (salinity 7.2 permillage) (Bengtsson 1977).	
Other information about bioaccumulation	Positive correlation between age (length, weight) and Cd of whole body of organisms has been noticed. When salinity increases accumulation of Cd decreases both in invertebrates and fish (forming of not bioavailable chloride complexes) (Broman et al. 1988).	
LD50 values to mammals in oral exposure, mg/kg	225	orl-rat (Lewis & Sweet 1984)
LC50 values to mammals in inhalation exposure, mg/m³	500	ihl-rat (Friberg et al. 1971)
TCLo values to mammals in inhalation exposure, mg/kg	0.08	ihl-man (Lewis & Sweet 1984)
Health effects	Toxic by inhalation of dust or fume. A carcinogen. Cadmium plating of food and beverage containers has resulted in a number of outbreaks of gastroenteritis (food poisoning). Soluble compounds of cadmium are highly toxic; however, ingestion usually induces a strong emetic action which minimizes the risk of fatal poisoning. Use as fungicide may be restricted (Sax & Lewis 1987).	
Effects on plants	Height growth and dry weight accumulation of 6 week old soybeans (Glycine max) were severely reduced by 4 ppm CdCl2 in quartzsand culture (Chaney et al. 1977). Two cultivars of cotton (Gossypium spp.) were grown in solution culture. CdC04 was phytotoxic at 0.00001 M (Rehab & Wallace 1978). Soybean seeds (Glycine max) were planted in acid-washed sand. Beginning 5 days after seed germination the sand was saturated with metal solutions; Cd at 1 ppm caused reductions in stem and foliage dry weights (leaves and stems contained 0.00285 mg Cd/g) (Vesper & Weidensaul 1978).	
LC50 values to algae, mg/l	2.1	Chlorella pyrenoidosa (Brauwers 1982)
	0.05	Cd2+, Cylindrotheca closterium (Piotrowski & Coleman 1980)
EC50 values to algae, mg/l	3	96hr, rpd, Navicula incerta (Rachlin et al. 1983)
	0.11	96hr, rpd, Chlorella saccharophila (Rachlin et al. 1982)

LC50 values to crustaceans, mg/l	1.32	Cd(II), 96hr, mbt, Asellus aquaticus
	4.58	Cd(II), 48hr, mbt, Asellus aquaticus (Martin & Holdich 1986)
		d, Daphnia magna
	0.065	48hr, without food, D.magna (Biesinger & Christensen 1972)
	0.0401	96hr, Gammarus lacustris (DeMarch 1988)
EC50 values to crustaceans, mg/l	0.0007	21d, rpd, Daphnia magna (Biesinger & Christensen 1972)
	0.0035	14d, Daphnia magna (Elnabarawy et al. 1986)
LOEC values to crustaceans, mg/l	0.00017	21d, rpd, Daphnia magna (Biesinger & Christensen 1972)
LC50 values to fishes, mg/l	0.004	sfd, 96hr, Morone saxatilis
	0.01	hrd
	0.075	1%. salt water (Palawski et al. 1985)
	0.0011	96hr, Oncorhynchus tshawytscha (Finlayson & Verrue 1982)
	2.3–2.5	96hr, Lepomis macrochirus (Bishop & McIntosh 1981)
	3.5–11.2	96hr, Branchydanio rerio (Bresch 1982)
	0.016–0.017	act, Salmo gairdneri (Majewski & Giles 1981)
	0.14	28d, Salmo gairdneri (Birge et al.1980)
	0.005	25d, Salmo (Nilsson & Wallgren 1987)
	18.5	96hr, Channa punctatus (Shukla & Pandey 1988)
LOEC values to fishes, mg/l	0.057	eggs, schr, Pimephales promelas (Pickering & Gast 1972)
	0.08	srv, grw, chr, Lepomis macrochirus (Eaton 1974)
	0.0034	srv, chr, Salvelinus fontinalis (Benoit et al. 1976)
	0.004	grw, juv, m Salvelinus fontinalis (Eaton et al. 1978)
	0.008	rpd, chr, Platichthys flesus (Spehar 1976)
	0.017	srv, chr, Platichthys flesus (McKim 1977)
	0.017	srv, chr, Branchydanio rerio (Bresh 1982)
	0.012	srv, juv, Catostomus commersoni
	0.012	srv, juv, Salmo trutta m. lacustris
	0.012	srv, juv, Oncorhynchus kisutch
	0.013	srv, juv, Esox lucius (Eaton et al. 1978)
NOEC values to fishes, mg/l	0.037	eggs, schr, Pimephales promelas (Pickering & Gast 1972)
	0.031	srv, grw, chr, Lepomis macrochirus (Eaton 1974)
	0.0017	srv, chr, Salvelinus fontinalis (Benoit et al. 1976)
	0.001	grw, juv, m Salvelinus fontinalis (Eaton et al. 1978)
	0.004	rpd, chr, Platichthys flesus (Spehar 1976)
	0.003	srv, chr, Plarichthys flesus (McKim 1977)
	0.001	srv, chr, Branchydanio rerio (Bresh 1982)
	0.004	srv, juv, Catostomus commersoni
	0.004	srv, juv, Salmo trutta m. lacustris
	0.004	srv, juv, Oncorhynchus kisutch
	0.004	srv, juv, Esox lucius (Eaton et al. 1978)

Effects on the physiology of water organisms	Pimephales promelas, 0.00028 mg/l, physiological effect (Benson & Birge 1987). Salmo gairdneri, 360d, 0.009 mg/l, biochemical effect (Krezoski et al. 1988). Salvelinus fontinalis, 0.00002–2.000 mg/l, growth effect, hatchability effect (Gingerich et al. 1988). Tilapia mossambica, 7–42d, 100 mg/l, hematological effect (Ruparelia et al. 1987).
Other information about water organisms	LC50 (96hr), 0.872 mg/l, Lymnea acuminata (Khangarot et al. 1982). Procambarus clarkii: > 0.1 mg/l, 4 days, enzyme effect (change in enzyme activity) (Almar et al. 1987). Dinoflagellate; inhibited growth, 0.001 mg/l, Cd^{2+} (Nilsson & Wallgren 1987). Daphnia, inhibition of ALA-D activity, 0.0001 mg/l (Berglind 1985). Algae, 14d, 0.100 mg/l, biomass effect (Kerrison et al. 1988). Channa punctatus, 13d, 3.5 mg/l, growth effect (Shukla & Pandey 1988). Daphnia magna, 28d, lethal effect, 0.005 mg/l (Dillon & Suedel 1987). Gambusia affinis, mortality, 2d, 6.7 mg/l (Chagnon & Guttman 1988). Invertebrates, 14d, 0.001–0.003 mg/l, biomass effect (Lawrence & Holoka 1987).

408 • Cadmium chloride

10108-64-2

Sumformula of the chemical	$CdCl_2$	
Water solubility, mg/l	1400000 20 °C	
Mobility	Cd appears mainly as chloride complexes ($CdCl^+$ and $CdCl_2$) in brackish and marine waters (Zirino & Yamamoto 1972).	
LD50 values to mammals in oral exposure, mg/kg	88	orl-rat (Christensen 1973)
Effects on arthropods	Chironomus riparius: LC50, 0.42 days, 1.35–325.0 mg/l LC50, 1 days, 2.1–2000.0 mg/l LC50, 2 days, 45.0–725.0 mg/l LC50, 4 days, 13.0–54.0 mg/l (Williams et al. 1986).	
LOEC values to algae, mg/l	0.05	$CdCl_2$, Selenastrum (Bartlett et al. 1974)
LC50 values to crustaceans, mg/l	0.195	96hr, Macrobrachium lamarrei (Murti & Shukla 1984)
	18.4–58.5	4 days,Procambarus clarkii (Del Ramo et al. 1987)
	10.2	96hr, Orconectes nais (Phipps & Holcombe 1985)
	0.065	48hr, Daphnia (Biesinger & Christensen 1972)
	3.3–10	48hr, Crangon, marine water
	1.2	48hr, Crangon, brackish water (Portmann & Wilson 1971)
EC50 values to crustaceans, mg/l	4.58	2d, mbt, Asellus aquaticus
	1.32	4d, mbt, Asellus aquaticus
	34.6	2d, mbt, Crangonyx pseudogracilis
	1.7	4d, mbt, Crangonyx pseudogracilis (Martin & Holdich 1986)
	2.6	21d, rpd, Daphnia magna (Knowles & McKee 1987)

LC50 values to fishes, mg/l	5.08	96hr, flow-through, Salvelinus fontinalis (Holcombe et al 1983)
	2.20–3.51	mg/l, 4d, Pimephales promelas (Sherman et al. 1987)
	3.3 –100 mg/l	2 days, Salmo gairdneri (Shazili & Pascoe 1986)
	1.5	96hr, Pimephales promelas
	0.003	96hr, Salmo gairdneri
	0.748	96hr, Carassius auratus
	4.48	96hr, Ictalurus punctatus
	6.47	96hr, Lepomis macrochirus (Phipps & Holcombe 1985)
	39	96hr, Barbus arulius (Shivaraj & Patil 1988)
	1.41	24hr, Salmo gairdneri (Zinkl et al. 1987)
EC50 values to fishes, mg/l	0.002	13d, srv, Oryzias latipes (Canton & Slooff 1979)

Effects on the physiology of water organisms	Carassius auratus, 10 days, 0.004 mg/g, biochemical effect (change in physio-chemical process including glycogen uptake, cholesterol levels and lipid analysis) (Carpene et al. 1987). Daphnia magna, 4 days, 0.0008 mg/g, biochemical effect (Knowles & McKee 1987). Oryzias latipes, 0.04 days, 10 mg/l, delayed mortality in recovery water (Michibata et al. 1987). Anodonta anatina, 21–112d, 0.029 mg/l, histological effect; Anodonta cygnea, 21–112d, 0.029 mg/l, histological effect (Hemelraad & Herwig 1988). Barbus arulius, 1–4d, 40.0 mg/l, oxygen consumption effect (Shivaraj & Patil 1988). Carassius auratus, 273d, 0.010 mg/l, physiological effect (Suzuki et al. 1987). Clarias batrachus, 14d, 1.0 mg/l, biochemical effect (Jana & Sahana 1988). Salmo gairdneri, 1d, 0.250 mg/l, biochemical effect (Zinkl et al. 1987).
Other information about water organisms	EC50 (100d), 0.65 mg/l, srv, Xenopus laevis (Canton & Slooff 1979). EC20 (28d), 0.0009 mg/l, protozoa (Cairns et al. 1986). LC50, 0.093 mg/l, 96hr, snail (Phipps & Holcombe 1985) Acetabularia, marine, inhibited cell growth, 0.001 mg/l (CdCl+ + Cd2+) (Karez et al. 1989). Capitella capitata, LC50, 28 weeks, 0.43 mg/l, CdCl2 (Reish et al. 1976). Daphnia, rpd, 3 weeks, 0.010 mg/l, CdCl2 (Biesinger & Christensen 1972). Salmo gairdneri, rpe, 0.001–0.002 mg/l, CdCl2 (Brown 1975). Anabaena variabilis, Chlorella vulgaris, 7d, 0.0000035 M, effect on population growth (Kosakowska et al. 1988).

409 • Cadmium(II)oxide

1306-19-0

Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).

410 • Cadmium nitrate

10325-94-7

Synonyms	Nitric acid, cadmium salt Cadmium dinitrate
Sumformula of the chemical	CdN2O6 * Cd(NO3)2
Use	Colouring glass and porcelain; laboratory reagent; cadmium salts. Photographic emulsions. Manufacturing light sensitive paper; chemicals production Ni-Cd batteries.

State and appearance	Prismatic white needles; hygroscopic.
Molecular weight	236.42
Vapour density (air=1)	2.455
Water solubility, mg/l	1500000 20 °C (Anon. 1989)
Melting point, °C	350
Boiling point, °C	132
Other information about degradation	Natural CO2 will slowly reduce concentration (Sax 1986).
Other information about metabolism	Cd content of livers and kidneys increased in direct proportion to intake. Kidneys retained 2–3 times the amount retained by the liver. Shellfish concentration Cd 900–1600 times (Sax 1986).
Health effects	Emphysema from Cd salt dusts, itai-itai disease (Sax 1986). Strong irritant. Affects central nervous system. Poor warning properties. Cadmium salts cause cramps, nausea, vomiting and diarrhea. Inflammation of mucous membrane. Headache. Oral ingestion has led to a number of human deaths. Acute poisoning causes lung damage; chronic poisoning damages kidneys, lungs, bones, causes blood changes. Symptoms include dark urine, dyspnea, chest pain (Sax 1986).
Effects on plants	Soybean, tomato, bushbean, and bahia grass plants were exposed to 0.1 g Cd per 6 or 7 inch pot (15–17 cm). The general symptoms included a red-brown discolouration of leaf veins, petioles and stems. Leaves cupped and rolled downward with puckering of intercostal laminae. Tomato leaves developed interveinal chlorosis and necrotic flecking, and yield reductions were observed. Iron foliar content decreased with increased Cd application in bahia grass and soybean. Manganese content decreased, due to increased Cd application in bahia grass but not in soybean (Sax 1986).
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 0.08 mg/l (Bringmann & Kühn 1980a)
NOEC values to algae, mg/l	0.7 rpd, schr, Selenastrum capricornutum (Slooff et al. 1983)
LC50 values to crustaceans, mg/l	0.047 48hr, Daphnia magna 0.14 48hr, Daphnia pulex 0.2 48hr, Daphnia cucullata (Canton & Adema 1978) 0.5 48hr, Asellus aquaticus (Slooff 1983) 0.08 48hr, Gammarus pulex (Slooff 1983)
EC50 values to crustaceans, mg/l	0.078 96hr, Homarus americanus 0.14 48hr, Daphnia pulex 0.2 48hr, Daphnia cucullata 0.042–0.055 48hr, Daphnia magna (Sax 1986)
LC50 values to fishes, mg/l	0.15 48hr, Salmo gairdneri (Slooff et al. 1983) 0.056 Cd, act, Poecilia reticulata 0.0066 Cd, 96hr, Salmo gairdneri (Sax 1986) 0.0066 96hr, flow-through, Salmo gairdneri (Hale 1977)

Effects on the physiology of water organisms	Selenastrum capricornutum, 0.13–4 days, 0.002–0.004 mg/l; growth effect (measurable change in length and/or weight (Thompson et al. 1987). Cyprinus carpio, hematological effect, 3.75d, 11 mg/l (Beena & Viswaranjan 1988). Lamellidens marginalis, physiological effect, 1d, 2 mg/l (Radhakrishnaiah 1988). Selenastrum capricornutum, population growth effect, photosynthesis effect, 4d, 0.002–0.008 mg/l (Thompson et al. 1987). Tilapia aurea, growth effect, mortality, 112d, 0.014–0.052 mg/l (Papoutsoglou & Abel 1988).
Other information about water organisms	2.7 mg/l, flatworm (Polycelis nigra), toxic threshold concentration. – 0.42 mg/l, stickleback, toxic threshold concentration. – 0.2 mg/l as Cd, stickleback, lethal concentration limit, 15–18 °C. – 0.7 mg/l as Cd, stickleback, survived. – 0.056 mg/l as Cd, guppy, LD50 (Sax 1986). LC50, 48hr, 6.5 mg/l, Tubificidae LC50, 48hr, > 56 mg/l, Chironomus gr. thummi LC50, 48hr, 4.2 mg/l, Erpobdella octoculata LC50, 48hr, 1.6 mg/l, Lymnaea stagnalis LC50, 48hr, > 56 mg/l, Dugesia cf. lugubris LC50, 48hr, 1.6 mg/l, Hydra oligactis LC50, 48hr, > 56 mg/l, Corixa punctata LC50, 48hr, > 56 mg/l, Ischura elegans LC50, 48hr, 49 mg/l, Nemoura cinerea LC50, 48hr, 56 mg/l, Cloeon dipterum (Slooff 1983) Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 0.031 mg/l protozoa (Entosiphon sulcatum): 0.011 mg/l (Bringmann & Kühn 1980a)
Other information	Air pollution: high (Sax 1986).

411 • Cadmium sulfate

10124-36-4

LC50 values to crustaceans, mg/l	5.3 1.5	1d, Daphnia magna 2d, Daphnia magna (Khangarot et al. 1987)
EC50 values to crustaceans, mg/l	4.66 1.88	1d, mbt, Daphnia magna 2d, mbt, Daphnia magna (Khangarot & Ray 1987)
LC50 values to fishes, mg/l	1.7 126	96hr, Branchydanio rerio (Dave et al. 1981) 96hr, Channa punctata (Srivastava Mishra 1979)
Effects on the physiology of water organisms	Salmo gairdneri, 4 days, 0.750 mg/l, enzyme effect (change in enzyme activity) (Castren & Oikari 1987). Spirulina platensis, 0.25 days, 0.010 mg/l, photosynthesis effect (change in plant productivity indicated by change in 14C or CO2 uptake or oxygen consumption) (Azeez & Banerjee 1987).	
Effects on the reproduction of water organisms	Pimephales promelas, 0.014 mg/l, CaSO4, effects on reproduction (Pickering & Gast 1972).	

412 • Caffeine

58-08-2

Synonyms	Theine Methyltheobromine 1,3,7-trimethylxanthine

Sumformula of the chemical	C8H10N4O2 . H2O * bicyclic compound	
Use	Beverages; medicine.	
Water solubility, mg/l	13500 455500	at 16 °C at 65 °C
Melting point, °C	236.8	
Log octanol/water coefficient, log Pow	-0.07	
LD50 values to mammals in oral exposure, mg/kg	200	orl-rat (McCann et al. 1975)
Mutagenicity	Mutagenicity in the Salmonella test: none; < 0.002 revertant colonies/nmol; < 70 revertant colonies at 6 mg/plate (McCann et al. 1975).	
LD50 values to birds in oral exposure, mg/kg	316 500	orl-Agelaius phoeniceus orl-Sturnus vulgaris (Schafer et al. 1983)

413 • Calcium and calcium compounds 7440-70-2

LC50 values to crustaceans, mg/l	330 52 464 580	21d, Daphnia magna 48hr, without food, Daphnia magna 48hr, with food, D.magna (Biesinger & Christensen 1972) 96hr, Nitocra spinipes (Bengtsson 1978)
EC50 values to crustaceans, mg/l	220	rpd, 21d, Daphnia magna (Biesinger & Christensen 1972)
LOEC values to crustaceans, mg/l	116	rpd, 21d, Daphnia magna (Biesinger & Christensen 1972)

414 • Calcium chloride 10043-52-4

Sumformula of the chemical	CaCl2	
Molecular weight	110.98	
LD50 values to mammals in oral exposure, mg/kg	1940 1000	orl-mus orl-rat (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	25 245 264 42 823 2630	ims-rat ipr-mus ipr-rat ivn-mus scu-mus scu-rat (Sweet 1987)

LDLo values to mammals in non-oral exposure, mg/kg	110	ipr-dog
	249	ivn-cat
	274	ivn-dog
	161	ivn-rat
	274	ivn-rbt
	249	scu-cat
	274	scu-dog
	472	scu-rbt
		(Sweet 1987)
TDLo values to mammals in oral exposure, mg/kg	112000	orl-rat, tumorigenic (Sweet 1987)
Mutagenicity	Mutation data: cyt, rat, Ascites tumor, 3500 mg/kg; sns, rat, ipr, 2.5 mmol/kg; sin, smc, 200 mmol/l (Sweet 1987).	
Effects on amphibia	LDLo, 666 mg/kg, frog (Sweet 1987).	

415 • Calcium di-trichloroacetate 21348-16-3

Sumformula of the chemical	C4O4Cl6Ca	
Water solubility, mg/l	478000	(MITI 1992)
Melting point, °C	100	(MITI 1992)
Total degradation in water	Biodegradation: 21.0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.3–0.9	6w, Cyprinus carpio, conc 0.2 mg/l
	< 3.0	6w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 1000	48, Oryzias latipes (MITI 1992)

416 • Calcium(II) nitrate 10124-37-5

Sumformula of the chemical	N2O6.Ca	
Molecular weight	164.1	
LD50 values to birds in oral exposure, mg/kg	> 99	orl-Agelaius phoeniceus (Schafer et al. 1983)

417 • Camphene 79-92-5

Water solubility, mg/l	4.6	(MITI 1992)
Melting point, °C	51.2	(MITI 1992)
Boiling point, °C	160	(MITI 1992)
Log octanol/water coefficient, log Pow	> 3.90	(MITI 1992)

Total degradation in water	Biodegradation: 1–4% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	432–922 606–1290	8w, Cyprinus carpio, conc 0.015 mg/l 8w, Cyprinus carpio, conc 0.0015 mg/l (MITI 1992)
LD50 values to birds in oral exposure, mg/kg	> 96	orl-Agelaius phoeniceus (Schafer et al. 1983)
LC50 values to crustaceans, mg/l	22	48hr, Daphnia magna (LeBlanc 1980)
LC50 values to fishes, mg/l	2.03	48hr, Oryzias latipes (MITI 1992)

418 • Camphor

76-22-2

Synonyms	Gum camphor 2-Camphanone	
Use	Odourant/flavourant in household; pharmaceutical and industrial products; plasticizer for cellulose esters and ethers; insect repellant and incense manufacturing; lacquers and varnishes; explosives; embalming fluid; plastics manufacturing; chemical intermediate.	
State and appearance	Colourless or white crystals.	
Odour	Quality: penetrating aromatic odour. Odour Index: at 20 °C: 40 (Verschueren 1983).	
Specific gravity (water=1)	0.99	
Vapour pressure, mmHg	1 400 700	at 41.5 °C at 182 °C at 209.2 °C
Melting point, °C	174–179 °C	
LC50 values to fishes, mg/l	110	96hr, Pimephales promelas (Mattson et al. 1976)
Other effects on aquatic ecosystems	Reduction of amenities: Threshold Odour Concentration in water at room temperature: 1.29 ppm, range 0.25–3.83; 20% of population still able to detect odour at 0.33 ppm 10% of population still able to detect odour at 0.041 ppm 1% of population still able to detect odour at 0.0092 ppm 0.1% of population still able to detect odour at 0.021 ppm (Lillard et al. 1975).	
Other information	Manufacturing source: organic chemical industry, wood processing industry. Natural sources (water and air): major component of pine oil (leaves, twigs, stems of camphor tree of China, Formosa, Japan); present in forest runoff.	

419 • Capacitor 21

66419-38-3

LC50 values to fishes, mg/l	0.002 0.002	23days, embryo, Salmo gairdneri 96hr, larvae, Salmo gairdneri (Birge et al. 1979)
	0.0052 0.0015	4 days, Ictalurus punctatus 4 days, Micropterus salmoide (Birge et al. 1978)

420 • n-Capric acid

334-48-5

Synonyms	Decanoic acid n-Decoic acid n-Decylic acid	
Sumformula of the chemical	CH3(CH2)8COOH	
Use	Esters for perfumes and fruit flavours, base for wetting agents; intermediate; plasticizer.	
Odour	Threshold Odour Concentration: 0.014 mg/m³ = 1.96 ppb (Stockham et al. 1969). Threshold Odour Concentration: detection: 0.05 mg/m³ recognition 0.08–0.09 mg/m³ (Verschueren 1983).	
Molecular weight	172.26	
Specific gravity (water=1)	0.886	at 40/4 °C
Vapour pressure, mmHg	1	at 125 °C
Melting point, °C	31.5	
Boiling point, °C	268–270	
pKa	4.9	est. (Sangster 1989)
Log octanol/water coefficient, log Pow	4.09	(Sangster 1989)
Other information about water organisms	Lepomis macrochirus; chemical is too insoluble in water to be toxic (Dowden 1960).	

421 • Caproic acid

142-62-1

Synonyms	Hexanoic acid n-Hexoic acid Butylacetic acid n-Caproic acid Capronic acid n-Hexanoic acid Pentiformic acid Pentylformic acid	
Sumformula of the chemical	C6H12O2	
State and appearance	Oily liquid.	
Odour	Characteristic: like limburger cheese.	
Molecular weight	116.2	
Specific gravity (water=1)	0.945	at 0/0 °C
Vapour density (air=1)	4.01	

Conversion factor, 1 ppm in air=	4.83	mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.21	ppm
Vapour pressure, mmHg	0.2 1	at 20 °C at 70 °C
Water solubility, mg/l	11000	
Melting point, °C	-6– -2	
Boiling point, °C	204–208	
pKa	4.87	(Sangster 1989)
Log octanol/water coefficient, log Pow	1.92	(Sangster 1989)
LD50 values to mammals in oral exposure,mg/kg	6440 5000 3000	orl-rat (Patty 1967) orl-mus orl-rat (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	3180 1725 3180 4635 630	ipr-mus ivn-mus scu-mus skn-gpg skn-rbt (Sweet 1987)
LC50 values to mammals in inhalation exposure,mg/m^3	4100	ihl-mus (Sweet 1987)
Other information about mammals	Skin and eye irritation data: skin, rbt, 10 mg, 24hr open, mild; skin, rbt, 465 mg open, mild; eye, rbt, 0.695 mg, severe (Sweet 1987).	
Mutagenicity	Mutation data: cytogenetic analysis: non-mammalian, cell types, 10 mmol/l; test systems (other): non-mammalian, cell types, 10 mmol/l (Sweet 1987).	
LC50 values to crustaceans, mg/l	22	24hr, Daphnia magna (Verschueren 1983)
LC50 values to fishes, mg/l	88	96hr, Pimephales promelas (Mattson et al. 1976)

422 • Caprolactam

105-60-2

Synonyms	ε-Caprolactam Cyclohexanoneisooxime	
Use	Nylon manufacturing and processing; manufacturing of plastics, bristles, films, coatings, synthetic leather, plasticizers and paint vehicles; cross linking agent for curing polyurethanes; synthesis of amino acid lysine.	
Odour	Threshold Odour Concentration: 0.3 mg/m^3 = 63 ppb (Verschueren 1983).	
Water solubility, mg/l	> 2000	(MITI 1992)
Vapour density (air=1)	3.91	
Conversion factor, 1 ppm in air=	4.7	mg/m^3

Conversion factor, 1 mg/m³ in air=	0.21	ppm
Vapour pressure, mmHg	0.001 0.0035	at 20 °C at 30 °C
Melting point, °C	68–70	(MITI 1992)
Boiling point, °C	139	(MITI 1992)
Total degradation in water	Biodegradation: 82% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
Other information about water organisms	Catfish: no effect: 1 g/l, 30 days catfish: toxic: 5 g/l after 18hr catfish: toxic: 10 g/l after 10hr (Meinck 1970).	
Other effects on aquatic ecosystems	Reduction of amenities: Threshold Odour Concentration in water at room temperature: 59.7 ppm, range 36.0–100 ppm, 8 judges; 20% of population still able to detect odour at 25 ppm 10% of population still able to detect odour at 16 ppm 1% of population still able to detect odour at 3.8 ppm 0.1% of population still able to detect odour at 0.92 ppm (Lillard et al. 1975). Water quality: 1.0 mg/l affects the self purification (Verschueren 1983); nitrification decreases from 100 mg/l onwards (Meinck 1970).	

423 • Caprylic acid

124-07-2

Synonyms	Octanoic acid n-Octoic acid n-Octylic acid	
Sumformula of the chemical	CH3(CH2)6COOH	
State and appearance	Colourless liquid or solid.	
Odour	Characteristic, unpleasant, irritating. In water: Threshold Odour Concentration: detection: 3.0 mg/kg (Cherkinski 1961).	
Molecular weight	144.21	
Specific gravity (water=1)	0.91	at 20/4 °C
Vapour density (air=1)	5	
Conversion factor, 1 ppm in air=	5.994	mg/m³
Conversion factor, 1 mg/m³ in air=	0.167	ppm
Vapour pressure, mmHg	1	at 92 °C
Water solubility, mg/l	2500	at 100 °C
Melting point, °C	16	
Boiling point, °C	237	
pKa	4.89	(Sangster 1989)
Log octanol/water coefficient, log Pow	3.05	(Sangster 1989)

Effects on the physiology of mammals	Dog: oral doses: 1–5% in diet causes diarrhea (Patty 1967).
Other information about water organisms	Lepomis macrochirus: chemical is too insoluble in water to be toxic (Dowden 1960).

424 • Captan

133-06-2

Synonyms	N-((Trichloromethyl)thio)-4-cyclohexene-1,2-dicarboximide N-Trichloromethylthiotetrahydrophthalimide cis-N-((Trichloromethyl)thio)-4-cyclohexene-1,2-dicarboximide	
Use	Protectant-eradicant fungicide.	
State and appearance	White solid.	
Molecular weight	300.59	
Water solubility, mg/l	< 0.5, 20 °C	
Melting point, °C	175	
Log octanol/water coefficient, log Pow	2.35	
Half-life in soil, days	3	(Li et al. 1990)
LD50 values to mammals in oral exposure, mg/kg	9000 740	orl-rat (Anon. 1976) orl-rbt (Lewis & Sweet 1984)
Other information about mammals	In diet: no effect level from 2 years dietary tests on rats; 1000 mg/kg (Martin 1968).	
Carcinogenicity	Carcinogenic (McCann et al. 1975). NCI carcinogenesis bioassay completed: results positive, mus; results negative, rat (Lewis & Sweet 1984).	
Mutagenicity	Mutagenicity in the Salmonella test positive (without liver homogenate): 25 revertant colonies/nmol; 820 revertant colonies at 0.010 mg/plate (McCann et al. 1975).	
LD50 values to birds in oral exposure, mg/kg	100–104 > 100 > 100 > 100	orl-Agelaius phoeniceus orl-Passer domesticus orl-Quiscalus quiscula orl-Corvus brachyrhynchos (Schafer et al. 1983)
Effects on plants	Development of mycorrhizal fungi in roots of sour orange (Citrus aurantium) seedlings was reduced by spraying of soil with 9.0 kg captan (50%) /ha (Nemec 1980).	
LC50 values to crustaceans, mg/l	1.5	Daphnia pulex (Hashimoto & Nishiuchi 1981)
LC50 values to fishes, mg/l	0.04 0.25 0.3	48hr, Carassius auratus 48hr, Cyprinus carpio (Hashimoto & Nishiuchi 1981) 96hr, Rasbora heteromorpha (Tooby et al. 1975)
LOEC values to fishes, mg/l	0.04	srv, chr, Pimephales promelas (Hermanutz et al. 1973)
NOEC values to fishes, mg/l	0.017	rpd, grw, Pimephales promelas (Hermanutz et al. 1973)

425 • Carbaryl

63-25-2

Synonyms	1-Naphthyl-N-methylcarbamate 1-Naphthyl methyl carbamate Carbamine Dicarbam Hexavin Methylcarbamate 1-naphthol Methylcarbamic acid, 1-naphthyl ester N-methyl-α-naphthylcarbamate n-methyl-α-naphthylurethan Sevin Tricarnam
Sumformula of the chemical	C12H11N02
Use	Insecticide, pesticide.
State and appearance	White crystalline solid.
Molecular weight	201.24
Specific gravity (water=1)	1.232 at 20 °C
Vapour pressure, mmHg	< 0.005 mm, 26 °C
Water solubility, mg/l	100 (MITI 1992)
Melting point, °C	142 (MITI 1992)
Photochemical degradation in water	direct photolysis *pH* — *half-life, days* 5 — 6.6 7 — 6.6 9 — - (Verschueren 1983).
Hydrolysis in water	hydrolysis pH — half-life, days 5 — 1500 7 — 15 9 — 0.15 Calculation based on neutral and alkaline hydrolysis assuming pseudo-first-order kinetics (Verschueren 1983).
Half-life in soil, days	22 (Li et al. 1990)
Aerobic degradation in soil	Biolysis by bacteria: half-life: > 30000 days (minimum value assuming a bacterial population of 0.1 mg/l (Wolfe et al. 1978).
Total degradation in water	Persistence in river water in a sealed glass jar under sunlight and artificial fluorescent light – initial concentration 0.010 mg/l *% of original compound found* after: 1hr — 90; 1wk — 5; 2wk — 0; 4wk — 0; 8wk — 0 (Eichelberger & Lichtenberg 1971). Biodegradation: 8*–65% by BOD (* 1-Naphtol was observed) period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

Other information about degradation	Biolysis by bacteria: half-life > 30000 days (Verschueren 1983)	
Bioconcentration factor, fishes	140	Ictalurus (Verschueren 1983)
Bioconcentration factor, crustaceans	260	(Verschueren 1983)
Bioconcentration factor, algae	4000	(Verschueren 1983)
Bioconcentration factor, other organisms	300 3600	snails Lemna sp. (Verschueren 1983)
LD50 values to mammals in oral exposure, mg/kg	250 500 850 150 250 212 710	orl-rat (Lewis & Sweet 1984) orl-rat, female orl-rat, male (Anon. 1976) orl-cat orl-gpg orl-mus orl-rbt (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	4000 2000 640 25 41.9 6717 1400 2000	skn-rat skn-rbt (Lewis & Sweet 1984) ipr-ham ipr-mus ivn-rat scu-mus scu-rat skn-rbt (Sweet 1987)
TDLo values to mammals in oral exposure, mg/kg	375 394 197 250 912 1370 5475 5640	orl-dog, 3-62d preg. specigic developmental abnormalities orl-dog, 1-63d preg. specigic developmental abnormalities orl-dog, 1-63d preg. effects on fertility orl-ham, effects on embryo of fetus orl-pig, 1-16w preg., eff. on fertility orl-rat, paternal effects orl-rat, maternal effects orl-rat, tumorigenic (Sweet 1987)
TDLo values to mammals in non-oral exposure, mg/kg	900 4176 80	6–15d, preg., scu-mus specific developmental abnormalities 6–14d, preg., scu-mus effects on embryo of fetus implant-rat, tumorigenic (Sweet 1987)
Other information about mammals	Dietary feeding; rats fed for 2 years on a diet containing 200 ppm suffered no ill effects (Martin 1968).	
Carcinogenicity	Carcinogenicity: negative (McCann et al. 1975).	

Mutagenicity	Mutagenicity in the Salmonella test: negative; < 0.008 revertant colonies/nmol < 70 revertant colonies at 2.0 mg/plate (McCann et al. 1975).
LD50 values to birds in oral exposure, mg/kg	56 orl-bwd (Lewis & Sweet 1984) 56.2–150 orl-Agelaius phoeniceus ≥ 100 orl-Passer domesticus (Schafer et al. 1983)
Effects on amphibia	LC50 (96hr), 55.34 ppm, tadpoles of Rana hexadactyla (Khangarot et al. 1985).
Effects on invertebrates	Invertebrates; 50 days, 1 mg/l, abundance effect (number of organisms in the same species changes) (Hanazoto & Yasuno 1987).
Effects on bees	Bees: 48hr, LC50: 3.8–4.5 ppm in food (Winterlin & Walker 1973).
Effects on arthropods	LC50 (96hr), 0.624 mg/l, Ranatra elongata (Shukla et al. 1982). NOEC (96hr), 0.0048 mg/l, Pteronarcys californica NOEC (96hr), 0.0017 mg/l, Pteronarcella badia NOEC (96hr), 0.0056 mg/l, Claassenia sabulosa (Sanders & Cope 1968). LC50 (30 days), 0.0022 mg/l; NOEC (30 days), 0.0013 mg/l; Acroneuria lycorias (Verschueren 1983). LC50 (30 days), 0.023 mg/l; NOEC (30 days), 0.0115 mg/l; Pteronarcys dorsata (Verschueren 1983). LC50 (30 days), 0.0027 mg/l; NOEC (30 days), 0.0018 mg/l; Hydropsyche bettoni (Verschueren 1983). Insect larvae: Chaoborus: 48hr, LC50: 0.296 ppm Cloeon: 48hr, LC50: 0.48 ppm (Verschueren 1983). Fourth instar larval Chironomus riparius: 24hr, LC50: 104.5 ppb (Estenik & Collins 1979). Rice-field spider (Oedothorax insecticeps): LD50: 840 ppm (Ishikura 1972).
Effects on microorganisms	Bacteria: Pseudomonas putida; inhibition of cell multiplication starts at > 50 mg/l (Bringmann & Kühn 1976).
LOEC values to algae, mg/l	0.03 Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to crustaceans, mg/l	0.00064 act, Daphnia pulex (Kenaga 1979) 0.006 48hr, Daphnia pulex (Shapiro 1979) 0.0326 96hr, Macrobrachium lamarrei (Shukla & Omkar 1984) 0.019 96hr, Macrobrachium lamarrei (Omkar & Shukla 1985) 0.029 96hr, Gammarus pulex (Bluzat & Seuge 1979) 0.007 96hr, Palaemon macrodactylus (Verschueren 1983) 0.74 act, Daphnia pulex (Frear & Boyd 1967) 0.05 act, Daphnia pulex (Hashimoto & Nishiuchi 1981) 0.00085 act, Daphnia pulex (Nishiuchi & Hashimoto 1967) 2 24hr, Daphnia magna 1 48hr, Daphnia magna (Bogacka & Groba 1980) 1 4d, Procambarus clarkii (Andreu-Moliner et al. 1986) 2.87 96hr, Orconectes nais (Phipps & Holcombe 1985)
EC50 values to crustaceans, mg/l	0.006 48hr, Daphnia pulex (Shapiro 1979)

NOEC values to crustaceans, mg/l	0.016	96hr, Gammarus lacustris
	0.026	96hr, Gammarus fasciatus (Sanders 1969)
	0.0056	96hr, Palaemonetes kanadiakensis
	0.0086	96hr, Orconectes nais
	0.24	96hr, Asellus brevicaudus
	0.0076	48hr, Simocephalus serrulatus (Sanders 1972)
	0.0064	48hr, Daphnia pulex
	0.005	63 days, Daphnia magna (Sanders & Cope 1966)
	0.008	chr, Daphnia (Biesinger 1973)
LC50 values to fishes, mg/l	0.86	96hr, Salmo gairdneri (Phipps & Holcombe 1985)
	0.76	96hr, Oncorhynchus kisutch
	6.8	96hr, Lepomis macrochirus
	13.2	96hr, Carassius auratus
	7.5	96hr, Cyprinus carpio
	4.3	96hr, Salmo gairdneri
	2	96hr, Salmo trutta m. lacustris
	0.75	96hr, Perca fluviatilis (Macek & McAllister 1970)
	3.4	24hr, Lepomis macrochirus
	3.5	96hr, Salmo gairdneri (Edwards 1977)
	13	48hr, Cyprinus carpio
	> 10	48hr, Carassius auratus (Hashimoto & Nishiuchi 1981)
	4.7	96hr, Lebistes reticulatus (Bogacka & Groba 1980)
	0.76	sfd, 96hr, Morone saxatilis, juv.
	2.3	1%. salt water, 96hr, Morone saxatilis, juv. (Palawski et al. 1985)
	11.2	act, Lepomis macrochirus
	4.34	act, Salmo gairdneri
	14.6	act, Pimephales promelas (Kenaga 1979)
	2	180 days, Channa punctatus (Saxena & Garg 1978)
	40	24hr, Gambusia affinis
	31.8	96hr, Gambusia affinis (Chaiyarach et al. 1975)
	13.51	24hr, Cyprinus carpio
	10.36	96hr, Cyprinus carpio (Bhattacharya et al. 1975)
	2.83	4d, Salmo gairdneri (McKim et al. 1987)
	3.7	96hr, Barbus ticto ticto
	2.4	48hr, Rasbora heteromorpha (Kemp et al. 1973)
	5.01	96hr, Pimephales promelas
	0.86	96hr, Salmo Gairdneri
	16.7	96hr, Carassius auratus
	12.4	96hr, Ictalurus punctatus
	6.97	96hr, Lepomis macrochirus (Phipps & Holcombe 1985)
LOEC values to fishes, mg/l	0.068	Pimephales promelas (Carlson 1972)

NOEC values to fishes, mg/l	0.21	srv, rpd, chr, Pimephales promelas
	0.3	chr, Pimephales promelas (Carlson 1972)
	9	96hr, Pimephales promelas
	0.21	6 months, Pimephales promelas
	0.68	6 months, srv, rpd, Pimephales promelas (Verschueren 1983)
	6.76	96hr, Lepomis macrochirus
	11.2	96hr, Lepomis microlophus
	6.4	96hr, Micropterus salmoides
	4.34	96hr, Salmo gairdneri
	1.95	96hr, Salmo trutta
	0.764	96hr, Oncorhynchus kisutch
	0.745	96hr, Perca flavescens
	15.8	96hr, Ictalurus punctatus
	20	96hr, Ictalurus melas (Macek & McAllister 1970)
Other information about water organisms	Algae: Microcystis aeruginosa: inhibition of cell multiplication starts at 0.03 mg/l (Bringmann & Kühn 1976). Crustacean: Cancer magister (Ducgeness crab): 6 ppb (egg/prezoeal) Prevention of hatching and molting (96hr) 10 ppb (zoea) Prevention of hatching and molting (96hr) 280 ppb (juvenile) Death or paralysis (96hr) 180 ppb (adult) Death or paralysis (96hr) (Verschueren 1983). Molluscs: Crassostrea gigas (Pacific oyster): 2200 ppb; 48hr, larvae; EC50 prevention of development to straight linge shell stage (Verschueren 1983). Mytilus edulis (bay mussel): 2300 ppb; 96hr, larvae; EC50 prevention of development to straight linge shell stage (Verschueren 1983). Salmo gairdneri; lethal threshold concentration (LT50): 5.167 mg/l; 0.57 days (McKim et al. 1987). LC50, > 27.0 mg/l, 96hr, snail, Phipps & Holcombe 1985.	

426 • Carbazole

86-74-8

Synonyms	Dibenzopyrrole	
Sumformula of the chemical	C12H9N	
EINECS-number	2016960	
Molecular weight	167.21	
Specific gravity (water=1)	1.1	18/4 °C
Vapour pressure, mmHg	400	at 323.0 °C
Melting point, °C	224.4	(MITI 1992)
Boiling point, °C	354.8	(MITI 1992)
pKa	-4	(Sangster 1989)
Log octanol/water coefficient, log Pow	3.72	(Sangster 1989)

C

Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Bioconcentration factor, crustaceans	115 Daphnia pulex, wet weight (Southworth et al. 1979)
Bioconcentration factor, fishes	69–241 6w, Cyprinus carpio, conc 0.05 mg/l 34–200 6w, Cyprinus carpio, conc 0.005 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	2.45 48hr, Oryzias latipes (MITI 1992)

427 • Carbendazim 10605-21-7

Synonyms	Methyl benzimidazol-2-yl carbamate (=MBC) 2-(Methoxycarbonylamino) benzinidazole 2-Benzimidazolecarbamic acid, methyl ester
Sumformula of the chemical	C9H9N3O2
Use	Fungicide.
Molecular weight	191.21
Water solubility, mg/l	60 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	0.6–1.1 6w, Cyprinus carpio, conc 0.02 mg/l < 1.5–3.5 6w, Cyprinus carpio, conc 0.002 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	6400 orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	2000 skn-rat (Lewis & Sweet 1984) 7320 ipr-rat (Lewis & Sweet 1984)
Effects on plants	Bavistin was applied to soil using 50% a.i. wettable powder: 0.020 grams of Bavistin available per plant caused decrease in chloroplast activity of the leaves of gherkin seedlings (Cucumis sativus L.) (van Wambeke et al. 1977). Carbendazim (100 µg/l) induced abnormalities in cell division in about 3% of cells in the root tips of onion (Allium cepa) after 4hr incubation (Richmond & Pring 1977).
LC50 values to algae, mg/l	0.34 48hr, Chlorella pyrenoidosa (Canton 1976)
EC50 values to algae, mg/l	0.34 48hr, rpd, Chlorella pyrenoidosa (Canton 1976)
LC50 values to crustaceans, mg/l	0.46 48hr, Daphnia magna (Canton 1976)

LC50 values to fishes, mg/l	0.36 1.8	96hr, Salmo gairdneri 48hr, Salmo gairdneri (Canton 1976)
	4	48hr, Oryzias latipes (MITI 1992)
Other information	Product from the metabolism of benomyl.	

428 • Carbetamex 16118-44-3

Synonyms	Carbetamide	
LC50 values to fishes, mg/l	165	96hr, Rasbora heteromorpha (Tooby et al. 1975)

429 • Carbofuran 1563-66-2

Synonyms	2,3-Dihydro-2,2-dimethylbenzofuran-7-yl-methylcarbamate 2,3-Dihydro-2,2-dimethyl-7-benzofuranylmethylcarbamate	
Use	Systemic insecticide widely used to control corn rootworms.	
State and appearance	White crystalline solid.	
Odour	Odourless.	
Molecular weight	221.3	
Specific gravity (water=1)	1.18	20/20 °C
Vapour pressure, mmHg	0.00002	33 °C
Melting point, °C	150–152	
Volatilization	Volatilization at 25 °C from soils in the laboratory: sandy loam: 0.5% after 60 days sand: 36.2% after 60 days (Caro et al. 1976).	
Half-life in soil, days	11–13 60–75	days, pH 6.5, technical carbofuran days, pH 6.5, granular formulation (Ahmad et al. 1979)
	40	(Li et al. 1990)
Half-life in water, days	11–13	calculated, pH 6.5, technical carbofuran (Verschueren 1983)
	60–75	calc., pH 6.5, granular formulation (Verschueren 1983)
Total degradation in soil	95% disappearance from the soil: 145–434 days (Caro et al. 1976).	
LD50 values to mammals in oral exposure, mg/kg	5.3	orl-rat (Lewis & Sweet 1984)
	11	orl-rat (Anon. 1976)
LD50 values to mammals in non-oral exposure, mg/kg	120 885	skn-rat skn-rbt (Lewis & Sweet 1984)
	10200	skn-rbt (Anon. 1976)

LD50 values to birds in oral exposure, mg/kg	0.415	orl-dck
	0.42	orl-bwd (Lewis & Sweet 1984)
	0.422	orl-Agelaius phoeniceus
	5.62	orl-Sturnus vulgaris
	1.33	orl-Passer domesticus
	1.33–3.16	orl-Quiscalus quiscula
	1.33	orl-Columba livia
	0.75	orl-Carbodacus mexicanus
	1.33	orl-Molothrus ater (Schafer et al. 1983)
Effects on amphibia	LC50 (96hr), 112.7 ppm, tadpoles of Rana hexadactyla (Khangarot et al. 1985).	
LC50 values to crustaceans, mg/l	0.547	96hr, Saccobranchus fossilis (Verma et al. 1982a)
LC50 values to fishes, mg/l	8.5	48hr, Salmo gairdneri,
	11	48hr, Cyprinus carpio
	3.4	48hr, Poecilia reticulata (Hejduk & Svobodova 1980)
	0.52	72hr, Gambusia affinis
	0.16	72hr, Lepomis cyanellus (Davey et al. 1976)
	0.26	96hr, Mystus vittatus
	0.18	96hr, Channa punctata (Verma et al. 1981)
	0.386	96hr, Cyprinodon variegarus (Jackson 1979)
	0.16	4d, Cyprinus carpio (Kulshrestha & Arora 1986)
	3.4	0.04, Lepidocephalus thermalis (Bakthavathsalam 1987)
LOEC values to fishes, mg/l	0.023	srv, schr, Cyprinodon variegetus (Parrish et al. 1977)
	0.049	srv, chr, Cyprinodon variegatus (Ward & Parrish 1980)
NOEC values to fishes, mg/l	0.015	srv, schr, Cyprinodon variegatus (Parrish et al. 1977)
Effects on the physiology of water organisms	Lepidocephalus thermalis; 1 mg/l, 0.5d, histological effect (presence of physical damage to tissues) (Bakthavathsalam et al. 1987).	

430 • Carbon dioxide   124-38-9

Synonyms	Carbonic acid gas	
	Carbonic anhydride	
	Dry ice	
Sumformula of the chemical	C02	
Molecular weight	44.01	
Henry's law constant, Pa x m^3/mol	2217	calc. (Yaws et al. 1991)
LCLo values to mammals in inhalation exposure, ppm	90000	ihl-hmn, ihl-mam, 5min (Sweet 1987)
TCLo values to mammals in inhalation exposure, ppm	550000	ihl-mus, 2hr, 3d male paternal effects
	550000	ihl-mus, 4hr, 6d male
LD50 values to birds in inhalation exposure, mg/m^3	394000	ihl-Agelaius phoeniceus
	469000	ihl-Sturnus vulgaris
	392000	ihl-Coturnix coturnix (Schafer et al. 1983)

431 • Carbondisulfide

75-15-0

Synonyms	Carbonbisulfide Carbon disulfide Carbon sulfide	
Sumformula of the chemical	CS_2	
Use	Manufacturing rayon, cellophane, carbon tetrachloride, rubber chemicals and flotation chemicals, soil disinfectants, electronic vacuum tubes; solvent (phosphorus, sulfur, bromine, iodine, selenium, fats, resins, rubbers); manufacturing grain fumigants, soil conditioners, herbicides; paper manufacturing; pharmaceutical manufacturing.	
State and appearance	Colourless liquid.	
Odour	Characteristic; vegetable sulfide, aromatic. Hedonic tone: slightly pungent. Odour Index: (100% recognition) 1600000 Human odour perception: non perception: 0.04 mg/m³; perception: 0.05 mg/m³ = 16 ppb Human reflex response: no responde: 0.03 mg/m³; adverse response: 0.04 mg/m³ (Verschueren 1983).	
Molecular weight	76.14	
Specific gravity (water=1)	1.263	at 20/4 °C
Vapour density (air=1)	2.64	
Conversion factor, 1 ppm in air=	3.17	mg/m³
Conversion factor, 1 mg/m³ in air=	0.315	ppm
Vapour pressure, mmHg	200 260 430	10 °C 20 °C 30 °C
Water solubility, mg/l	2300 2900	22 °C 20 °C
Melting point, °C	-110	
Boiling point, °C	46.3	
Log octanol/water coefficient, log Pow	1.84	
Henry's law constant, Pa x m³/mol	1946	calc. (Yaws et al. 1991)
Volatilization	Relative volatility (nBuAc=1) = 25.93	
Other information about degradation	Impact on biodegradation processes: 75% reduction of the nitrification process in activated sludge at 35 mg/l (Meinck et al. 1970).	
LD50 values to mammals in oral exposure, mg/kg	2125 2780 3188 2550	orl-gpg orl-mus orl-rat orl-rbt (Sweet 1987)
LDLo values to mammals in oral exposure, mg/kg	14	orl-hmn (Lewis & Sweet 1984)
LDLo values to mammals in non-oral exposure, mg/kg	186 400	unk-man (Lewis & Sweet 1984) ipr-gpg (Sweet 1987)

LCLo values to mammals in inhalation exposure, ppm	4000 2000 2000	30 min, ihl-hmn (Lewis & Sweet 1984) 5min, ihl-hmn, 5 min, ihl-mam (Lewis & Sweet 1987) 30 min, ihl-hmn (Lewis & Sweet 1984) 5 min, ihl-hmn, 5 min, ihl-mam (Lewis & Sweet 1987) 30 min, ihl-hmn (Lewis & Sweet 1984) 5min, ihl-hmn, 5 min, ihl-mam (Sweet 1987) 30 min, ihl-hmn (Lewis & Sweet 1984) 5 min, ihl-hmn, 5 min, ihl-mam (Sweet 1987)
TDLo values to mammals in oral exposure, mg/kg	2000 350 2100	orl-rat, 6–15d effects on embryo or fetus orl-rbt, 6–19d preg. effects on fertility orl-rbt, 6–19d preg. specific developmental abnormalities (Sweet 1987)
TCLo values to mammals in inhalation exposure, mg/kg	40 2000 200 10 100 100 0.03 600	ihl-man, paternal effects ihl-mus, 2hr, 1–21d preg. effects on fertility ihl-rat, 24hr, 1–21d preg. effects on fertility ihl-rat, 8hr, 1–22d preg. specific developmental abnormalities effects on newborn ihl-rat, 8hr, 1–22d preg. effects on newborn ihl-rat, 8hr, 1–21d preg. effects on embryo of fetus specific developmental abnormalities ihl-rat, 8hr, 1–22d preg. effects on newborn ihl-rat, 6hr, paternal effects (Sweet 1987)
Health effects	Man: severe toxic effects: 500 ppm = 1600 mg/m³, 60 min. symptoms of illness: 150 ppm = 480 mg/m³ unsatisfactory: > 10 ppm = 32 mg/m³ (Verschueren 1983).	
Mutagenicity	Mutation data: microbial mutation without S9: sat, 0.1 ml/plate; sister chromatid exchange: hmn, lym, 10.2 mg/l (Sweet 1987).	
EC50 values to algae, mg/l	21	96hr, rpd, Chlorella pyrenoidosa (Leeuwen et al. 1985)
LC50 values to crustaceans, mg/l	2.1	48hr, Daphnia magna (Leeuwen et al. 1985)
LC50 values to fishes, mg/l	4	96hr, Poecilia reticulata, Leeuwen et al. 1985
Other effects on aquatic ecosystems	Reduction of amenities: (Verschueren 1983).	faint odour: 0.0026 mg/l organoleptic limit: 1.0 mg/l

432 • Carbontetrachloride

56-23-5

Synonyms	Tetrachloromethane Methanetetrachloride Carbon chloride Perchloromethane	
Sumformula of the chemical	CCl4	
Use	Fire extinguisher manufacturing; dry cleaning operations; manufacturing of refrigerants, aerosols and propellants; manufacturing of chlorofluoromethanes; extractant; solvent; veterinary medicine; metal degreasing; fumigant; chlorinating organic compounds; intermediate.	
State and appearance	Colourless liquid.	
Molecular weight	153.81	
Specific gravity (water=1)	1.59	20 °C
Vapour density (air=1)	5.5	
Density, kg/m³	1594	20 °C
Conversion factor, 1 ppm in air=	6.39	mg/m³
Conversion factor, 1 mg/m³ in air=	0.16	ppm
Vapour pressure, mmHg	56 90 113	10 °C 20 °C 25 °C
Water solubility, mg/l	1160 785 800 800	25 °C 20 °C, 0.785–0.8 g/l (Anon. 1986b) (MITI 1992)
Melting point, °C	-22.99	(Suntio et al. 1988)
Boiling point, °C	76.54 76.7	(Anon. 1986b) (MITI 1992)
Log octanol/water coefficient, log Pow	2.64 2.73 2.7 2.64 2.83 2.62 2.73 2.64 2.64 2.64 2.83	20 °C, calculated (Anon. 1986b) (Anon. 1988) (Macy 1948) (Hansch & Leo 1979) (Chiou et al. 1977) (Banerjee et al. 1980) (Neely et al. 1974) (Mackay 1982) (Hawker & Connell 1985) (Sangster 1989)
Henry's law constant, Pa x m³/mol	1530 3080 2980	(Anon. 1988) exptl. (Gossett 1987) calc. (Yaws et al. 1991)
Volatilization	Measured half-life for evaporation from 1 ppm aqueous solution, still air and an average depth of 6.5 cm: at 25 °C: 28.8 min. (Verschueren 1983).	

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Mobility	Equilibrium distribution: *mass %* air 99.80 water 0.19 solid 0.02 (Anon. 1988). Theoretical distribution: > 99% air (Anon. 1989).
Photochemical degradation in air	Absorbs UV light in stratosphere where molecules break and form strongly reactive chloroatoms (IMOS 1975).
Other reactions in atmosphere	Stability in atmosphere 60–100 years (Borchers et al. 1983).
Hydrolysis in water	Hydrolysis half-life: 7000 years.
Half-life in water, days	0.002 = 28.8 min, measured evaporation from 1 ppm aqueous solution still air and an average depth of 6.5 cm, 25 °C (Verschueren 1983)
Aerobic degradation in water	Degrades very slowly in surface water (Ghisalba 1983).
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 199 mg/l sludge: 30 mg/l (MITI 1992).
Degradation and transformation products	Strongly reactive Cl is formed in stratosphere which break up ozone. In anaerobic conditions chloroform is formed (Anon. 1989).
Other information about degradation	Degradation of tetrachloromethane:

ENVIRONMENT	*CONC. mg/l*	*REDOX-COND.*	*TEMP. °C*	*DEGRADATION %/day*	*t1/2*	*REF.*
biofilm	0.017	methanogen	22	-	3.3 (1)	a
water	0.149	methanogen	35	100/16	< 8	b
water	0.054	denitrif.	25	63/14	10	c
water	0.076	denitrif.	25	69/14	12	c
biofilm+acetate	0.17	denitrif.	23	-	19 (1)	d
biofilm+acetate	0.17	sulfate reducing	23	-	35 (1)	d
biofilm+acetate	0.17	methanogen	23	-	11 (1)	d
soil	1.1	aerobic + natural gas		-	0.16	e
digested sludge	307.2	sulfate reducing		100/90	< 14	f
digested sludge	153.6	methanogen		100/90	< 14	f
active sludge	60.0	aerobic		76/14	< 7	f
water	5–10	aerobic	25	83/7	-	g
water (adapted)	5–10	aerobic	25	100/7	< 3	g

(1) Biomass concentration set to 0.100 mg/l.

a) Bouwer & McCarty 1985 b) Bouwer & McCarty 1983a
c) Bouwer & McCarty 1983 d) Bouwer & Wright 1987
e) Anon. 1987b f) Kästner 1986
g) Tabak et al. 1981 (Anon. 1987b).

Median stability in troposphere, based on the reaction with OH radicals is greater than 330 years (IMOS 1975).

Biologically catalysed hydrolysis (both aerobic and anaerobic) under methanogenic conditions – reductive dechlorination to trichloromethane (Kaare Jensen et al. 1987).

Metabolism in mammals	This compound is readily taken up by the lungs and more slowly by the gastrointestinal tract and skin. Distribution is dependent on the route of exposure, but is primarily to the lipid-rich tissues and bone-marrow. Most of a dose of tetrachloromethane is exhaled unchanged from the lungs, but some is metabolised by the liver. Early studies found that chloroform and to a lesser extent carbon dioxide were metabolites of tetrachloromethane. The first step in the biotransformation of tetrachloromethane is thought to involve the production of a trichloromethyl radical CCL3. This may then be converted to chloroform, dichloromethylcarbene, and phosgene or may react with molecular oxygen to form the highly reactive trichloromethyl peroxy radical CCl302. This radical may play an important role in the toxicity of tetrachloromethane to the liver (Fawell & Hunt 1988).
Bioconcentration factor, fishes	17.4 Salmo gairdneri (Verschueren 1983) 30 21d, Lepomis macrochirus (Anon. 1986b) 3.2–7.4 6w, Cyprinus carpio, conc. 0.01 mg/l 3.8–11 6w, Cyprinus carpio, conc 0.001 mg/l (MITI 1992)
Bioconcentration factor, algae	300 Chlorella (Geyer et al. 1984)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	2800 orl-rat (Lewis & Sweet 1984) 2920 orl-rat (Patty 1967) 5760 orl-gpg 8263 orl-mus 5760 orl-rbt (Sweet 1987) 1770 orl-rat (Anon. 1986b) 1000 orl-dog (Anon. 1986b) 6380 orl-rbt (Anon. 1986b) 2300 orl-rat (IARC 1979)
LD50 values to mammals in non-oral exposure, mg/kg	5070 skn-rat (Lewis & Sweet 1984) 1500 ipr-dog 572 ipr-mus 1500 ipr-rat 5840 ipr-rbt 31000 scu-mus 5070 skn-rat (Sweet 1987)
LC50 values to mammals in inhalation exposure, mg/m³	34500 ihl-mam (Sweet 1987)
LC50 values to mammals in inhalation exposure, ppm	9526 ihl-mus, 8hr 8000 ihl-rat, 4hr (Sweet 1987)
LDLo values to mammals in oral exposure, mg/kg	1000 orl-dog 43 orl-hmn (Lewis & Sweet 1984)
LDLo values to mammals in non-oral exposure, mg/kg	478 ipr-rbr 125 ivn-dog 300 scu-cat 3000 scu-rbt (Sweet 1987)

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LCLo values to mammals in inhalation exposure, ppm	38110	ihl-cat, 2hr ihl-dog ihl-gpg ihl-hmn
	14620	ihl-cat, 2hr ihl-dog ihl-gpg ihl-hmn
	20000	ihl-cat, 2hr ihl-dog ihl-gpg ihl-hmn
	1000	ihl-cat, 2hr ihl-dog ihl-gpg ihl-hmn (Sweet 1987)
TDLo values to mammals in oral exposure, mg/kg	2000	orl-rat, 7-8d preg. effects on fertility
	3000	orl-rat, 14d preg. effects on embryo or fetus
	7691	orl-rat, 10d male, paternal effects
	9250	orl-ham, tumorigenic
	4400	orl-mus, tumorigenic
	1700	orl-man, behavioral, gastrointest. lungs, thorax or respiration
	1800	orl-wmn, sense organs and special senses, behavioral (Sweet 1987)
TDLo values to mammals in non-oral exposure, mg/kg	71500	ipr-rat, 15d male, paternal effects
	5000	ipr-rat, 1d male, paternal effects
	2384	par-rat, 18d preg. effects on embryo or fetus specific developmental abnormalities
	305000	par-mus, tumorigenic
	15600	scu-rat, tumorigenic (Sweet 1987)
TCLo values to mammals in inhalation exposure, ppm	20	ihl-hmn (Lewis & Sweet 1984)
	300	ihl-rat, 7hr, 6-15d preg. effects on embryo or fetus specific developmental abnormalities
	250	ihl-rat, 8hr, 10-15d preg. effects on newborn
	20	ihl-hmn, gastrointestinal
	45	ihl-hmn, 3d, behavioral, gastrointest.
	317	ihl-hmn, 30 min, gastrointestinal

Effects on the physiology of mammals	Guinea pig; inhalation: slight increase in liver weight after a chronic exposure at 5 ppm (Patty 1967). Tetrachloromethane is of moderate acute toxicity in experimental animals. Lethan doses can induce death very rapidly by CNS depression or more slowly through massive liver damage. Hepatic changes are characterised by accumulation of fat, and cell necrosis in the centrilobular region. Tetrachloromethane also stimulates hepatic lipid peroxidation and depletes hepatic glutathione and glutathione-related enzymes. There is evidence to suggest that there is an age difference in susceptibility to tetrachloromethane hepatotoxicity in experimental animals but the mechanism of action of tetrachloromethane in the liver is not fully understood (Fawell & Hunt 1988). Acute studies have shown this compound to be toxic to the kidney and adrenal glands, and able to modify hepatic, adrenal and pulmonary mono-oxygenase activities. In subacute studies, high doses of tetrachloromethane were shown to be toxic to the testis in rats (Fawell & Hunt 1988).
Other information about mammals	Rat; inhalation: no effect: 3000 ppm, 6 min. inhalation: no effect: 800 ppm, 30 min. inhalation: no effect: 50 ppm, 7hr inhalation: no effect: 5 ppm, chronic exposure (Patty 1967). Skin and eye irritation data: skin, rabbit, 4 mg, mild; eye, rabbit, 2.2 mg, 30 s, mild; eye, rabbit, 500 mg, 24hr, mild (Sweet 1987). Rat, inhalation, 7hr, NOEC, 315 mg/m³ (IARC 1979).
Health effects	Man: severe toxic effects; 2000 ppm = 12800 mg/m³, 60 min. symptoms of illness: 500 ppm = 3200 mg/m³ unsatisfactory; > 50 ppm = 320 mg/m³ (Verschueren 1983). Indications that carbontetrachloride might cause liver cancer induction in humans (IARC 1979).
Carcinogenicity	Carcinogen (Verschueren 1983). Epidemiological data for carcinogenicity are sparse, though three cases of human liver cancer have been reported several years after poisoning with tetrachloromethane. However, a number of studies have shown that prolonged administration of high doses of tetrachloromethane by the oral or subcutaneous routes can induce liver tumours in rats, mice an hamsters (Fawell & Hunt 1988). Enough evidence for carcinogenicity in mammals (IARC 1979).

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Mutagenicity	Not Ames-mutagen (Verschueren 1983). Metabolites of tetrachloromethane have been reported to bind to hepatic nuclear and mitochondrial DNA in vivo, but bacterial mutagenicity tests heve largely proved negative. Tetrachloromethane also gave negative results for induction of unscheduled DNA synthesis in rat hepatocytes in vivo. However, positive results have been reported in yeast (Fawell & Hunt 1988). Mutation data: cyt, rat, scu, 31000 mg/kg; dnd, esc, 300 ppm; dnd, mam, lym, 1 mmol/l; dnd, mus, ipr, 0.367 mmol/kg; dnd, mus, liver, 0.010 mmol; dnd, mud, orl, 0.335 mmol/kg; dnd, rat, ipr, 0.367 mmol/kg; dnd, rat, scu, 31000 mg/kg; dnd, rat, liver, 3 mmol/l; DNA inhibition, mus, orl, 2000 mg/kg; dns, mus, orl, 100 mg/kg; mrc, asn, 5000 ppm; hma, mus, Ascites tumor, 6000 mg/kg; microbial mutation without S9, asn, 5000ppm, sat, 0.020 ml/l; otr, ham, emb, 0.5 mg/l; sin, asn, 5000 ppm (Sweet 1987). Negative in Ames test (IARC 1979).
Teratogenicity	The small number of studies that have looked at the reproductive toxicology of tetrachloromethane suggest that this compound is embryotoxic at high doses, but is not teratogenic (Fawell & Hunt 1988).
Effects on amphibia	LCLo, frog, 58000 mg/m³ (Sweet 1987). LC50, Buto fowleri, 92 mg/l, 3d; LC50, Buto fowleri, 2.82 mg/l, 4d; LC50, Rana catesbeiana, 1.50 mg/l, 4d; LC50, Rana catesbeiana, 0.90 mg/l, 4d; LC50, Rana palustris, 3.62 mg/l, 4d; LC50, Rana palustris, 2.37 mg/l, 4d. (Anon. 1986b)
Maximum longterm immission concentration in air for plants,mg/m³	3 VDI 2306
Maximum longterm immission concentration in air for plants,ppm	0.5 VDI 2306
Effects on microorganisms	Toxicity threshold (cell multiplication test): bacteria (Pseudomonas putida): 30 mg/l (Bringmann & Kühn 1980a). EC50 = 6 mg/l, 2 min, Photobacterium phosphoreum, EC50 = 5,6 mg/l, 5 min, Photobacterium phosphoreum (Anon. 1986b)
LOEC values to algae, mg/l	105 Microcystis aeruginosa (Weeks et al. 1979)
LC50 values to crustaceans, mg/l	35 48hr, Daphnia magna (LeBlanc 1980) 35.2 48hr, Daphnia magna (Anon. 1986b) 35 48hr, Daphnia magna (Anon. 1986b)

EC50 values to crustaceans, mg/l	721	24hr, Daphnia madna (Anon. 1986b)
	30	48hr, Daphnia magna
	31	24hr, Artemia (Abernethy et al.1986)
	1.7	16d, rpd, Daphnia (Hermens et al. 1984)
LC50 values to fishes, mg/l	4	96hr, Pimephales promelas
	1.97	96hr, Salmo gairdneri (Black et al. 1982)
	27	96hr, Lepomis macrochirus (Buccafusco et al. 1981)
	95–472	48hr, Leuciscus idus melanotus
	43.1	Pimephales promelas
	125	Lepomis macrochirus
	27.3	Lepomis macrochirus
	38	48hr, Lepomis macrochirus
	3.4	Pimephales promelas (Anon. 1986b)
	70	7d, Poecilia (Könemann 1981)
	45	48hr, Oryzias latipes (MITI 1992)
Other information about water organisms	EC50 (24hr), 830 mg/l, rpd, Tetrahymena pyriformis (Yoshioka et al. 1985). Toxicity threshold (cell multiplication test): algae (Microcystis aeruginosa): 105 mg/l (Bringmann & Kühn 1976) green algae (Scenedesmus quadricauda): > 600 mg/l protozoa (Entosiphon sulcatum): 770 mg/l protozoa (Uronema parduczi): 616 mg/l (Bringmann & Kühn 1980).	
Other information	Amount in troposphere: 3.7 Mt (1980) which is 18.5% of the total amount of organochlorides (Fabian 1986). Carbontetrachloride seem to be more effective than freons as catalyser for ozone break up (Anon. 1989).	

433 • Carbonylsulfide

463-58-1

Synonyms	Carbonoxysulfide	
Sumformula of the chemical	COS	
Odour	Characteristic; typical sulfide odour except when pure.	
Molecular weight	60.07	
Specific gravity (water=1)	1.24	at -87 °C
Vapour density (air=1)	2.1	
Melting point, °C	-138	
Boiling point, °C	-50.2	
Henry's law constant, Pa x m³/mol	5129	calc. (Yaws et al. 1991)

434 • Carbophenothion

786-19-6

Synonyms	S-(4-Chlorophenylthiomethyl)-0,0-diethylphosphorodithioate S-((p-Chlorophenylthio)methyl)-0,0-diethylphosphorodithioate S-(4-Chlorophenylthiomethyl)-diethylphosphorothiolothionate

Use	Insecticide, acaricide.
State and appearance	Off-white to amber liquid.
Odour	Mild mercaptan-like odour.
Molecular weight	342.87
Specific gravity (water=1)	1.275–1.3, at 20/20 °C
Vapour pressure, mmHg	0.0000003 20 °C
Water solubility, mg/l	< 40
Boiling point, °C	82
Log soil sorption coefficient, log Kom	4.66 (Sabljic 1987)
Total degradation in soil	50% degradation in soil occurs in 100 days or longer, depending on soil type (Martin 1968).
Total degradation in water	Persistence in river water: 0% of original compound found after 4 weeks (0.010 mg/l initial conc.) (Eichelberger & Lichtenberg 1971).
LD50 values to mammals in oral exposure, mg/kg	6.8 orl-rat (Lewis & Sweet 1984) 32.2 orl-rat (Nimmo et al. 1979)
LD50 values to mammals in non-oral exposure, mg/kg	27 skn-rat 1270 skn-rbt (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	6 orl-bwd (Lewis & Sweet 1984) 7.5 orl-Agelaius phoeniceus 5.62 orl-Sturnus vulgaris (Schafer et al. 1983)
LC50 values to crustaceans, mg/l	0.22 24hr, Daphnia magna 0.08 48hr, Daphnia magna (Ardo 1974) 0.003 96hr, Mysidopsis bahia (Anon. 1981) 0.00047 96hr, Penaeus duorarum (EPA 600/4-81-041) 0.0052 96hr, Gammarus lacustris (Sanders 1969) 0.0012 96hr, Palaemonetes kadiakensis 1.1 96hr, Asellus brevicaudus (Sanders 1972)
LC50 values to fishes, mg/l	0.0028 96hr, Cyprinodon variegetus (Anon. 1981) 0.0077 96hr, Lagodon rhomboides (EPA 600/4-81-04)

435 • Carboxin

5234-68-4

Synonyms	2,3-Dihydro-5-phenyl-carbamoyl-6-methyl-1,4-oxatine 5,6-Dihydro-2-methyl-1,4-oxathune-3-carboxanilide Vitavax DCMO
Use	Active ingredient in fungicides.
Molecular weight	235.32
Water solubility, mg/l	20
LD50 values to mammals in oral exposure, mg/kg	430 orl-rat (Lewis & Sweet 1984)

LD50 values to mammals in non-oral exposure, mg/kg	1050	skn-rat (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	24000 42.2	orl-ckn (Lewis & Sweet 1984) orl-Agelaius phoeniceus (Schafer et al. 1983)
LC50 values to crustaceans, mg/l	84.4	48hr, water flea (Pesticide Manual 1983)
LC50 values to fishes, mg/l	2 1.2	96hr, Salmo gairdneri 96hr, Lepomis macrochirus (Pesticide Manual 1983)

436 • Cartap

15263-52-2

Synonyms	S,S'-2-Dimethylaminotrimethylene-bis(thiocarbamate)	
Use	Insecticide.	
Molecular weight	492.59	
LD50 values to mammals in oral exposure, mg/kg	250 165	orl-rat orl-mus (Lewis & Sweet 1984)
LC50 values to crustaceans, mg/l	> 40	act, Daphnia pulex (Hashimoto & Nishiuchi 1981)
LC50 values to fishes, mg/l	0.78 1.1 1.3	48hr, Cyprinus carpio 48hr, Carassius auratus (Hashimoto & Nishiuchi 1981) 48hr, Cyprinus carpio (Pesticide Manual 1983)

437 • Catechol

120-80-9

Synonyms	o-Dihydroxybenzene 1,2-Dihydroxybenzene 1,2-Benzenediol Pyrocatechol o-Diphenol o-Hydroquinone o-Hydroxyphenol Oxyphenic acid o-Phenylenediol Catechin	
Sumformula of the chemical	C6H6O2	
Use	Preparation of dyes, pharmaceuticals, production of anti-oxidants for rubber and lubricatory oils. It is also used in photography, in rubber, in fur dyeing and in specialty inks as an agent for oxygen removal.	
State and appearance	Colourless leaflets.	
Molecular weight	110.12	
Specific gravity (water=1)	1.371	15 °C
Vapour density (air=1)	3.79	
Conversion factor, 1 ppm in air=	4.5	mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.22	ppm

Water solubility, mg/l	451000 20 °C
Melting point, °C	104–105 (MITI 1992)
Boiling point, °C	240–245 (MITI 1992)
Degradation point, °C	240
Log octanol/water coefficient, log Pow	0.88 1.01
Other chemical degradation processes	Ozonation: catechol + O_3 → o-quinone (Eisenhauer 1968). Autoxidation at 25 °C: t1/2: 447hr at pH 7.0 412hr at pH 9.0 (Moussavi 1979).
Total degradation in soil	Biodegradation: decomposition by a soil microflora: 1 day (Verschueren 1983).
Total degradation in water	Biodegradation: 83% by BOD substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
Other information about degradation	Routes for degradation of catechol by microorganisms: catechol I 'ortho'cleavage I 02 V cis, cis-muconate I V (+)-muconolactone I V 3-oxoadipate enol lactone I H20 V 3-oxoadipate I V 3-oxoadipyl CoA I V Acetyl-CoA + succinate catechol I 'meta'cleavage I 02 V 2-hydroxymuconic semialdehyde I H20 → HCOOH I V 2-oxo-pent-4-enoate I H20 V 4-hydroxy-2-oxovalerate I V acetaldehyde pyruvate (Verschueren 1983).
LD50 values to mammals in oral exposure, mg/kg	358 orl-rat 260 orl-mus 240 orl-mam (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	800 skn-rbt (Lewis & Sweet 1984)
LDLo values to mammals in oral exposure, mg/kg	100 orl-cat (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	> 100 orl-Agelaius phoeniceus (Schafer et al. 1983)
Effects on microorganisms	Bacteria: Escherichia coli: LD0: 90 mg/l (Meinck et al. 1970).

LC50 values to fishes, mg/l	8.9 96hr, Salmo gairdneri 3.5 96hr, Pimephales promelas (DeGraeve et al. 1980)
Other information about water organisms	Algae: Scenedesmus: LD0: 6 mg/l Protozoa: Vorticella campanula: LD0: 1.6 mg/l Paramaecium caudatum: LD0: 35 mg/l Arthropoda: Daphnia: LD0: 4 mg/l Fish: Trutta iridea: perturbation level: 3 mg/l Cyprinus carpio: perturbation level: 2.8 mg/l (Meinck et al. 1970). Goldfish: approximate fatal concentration: 14 mg/l, 48hr (McKee & Wolf 1963).
Other effects on aquatic ecosystems	Reduction of amenities: taste in fish (carp): 2.5 mg/l (Jones 1971) tainting of fish flesh: 2–5 mg/l (Verschueren 1983) odour threshold (detection): 8.0 mg/l (Verschueren 1983).

438 • Chandor *

8070-92-6

Active ingredients	trifluralin * 24%; linuron * 12%
Use	Herbicide.
LC50 values to fishes, mg/l	0.6 96hr, Rasbora heteromorpha (Tooby et al. 1975)

439 • Chinomethionat

2439-01-2

Synonyms	BAYER 36205 SAS 2074 Ss2074 Morestan * 6-Methyl-2,3-quinoxaline dithiocarbonate 6-Methyl-1,3-dithiolo(4,5-b)quinoxalin-2-one Chinomethionate
Sumformula of the chemical	C10H6N2OS2
Products containing the chemical	Morestan wettable powder (WP) * chinomethionat 250 g/kg (PESREG)
Use	Acaricide and fungicide for apple, strawberry, cucumber, rasberry, gooseberry, currants, tomato and ornamentals. (Morestan *) (PESREG)
Way to effect	Contact function. PESREG
Instruction for handling	Stable (full biological effect) at least for 24 months. (Morestan *) (PESREG)
State and appearance	Solid, crystalline, light yellow. Wettable powder (Morestan *) (PESREG)
Particle size, mm	0.04 maximum refuse to the sieve: 5% 0.071 maximum refuse to the sieve: 0.01% (PESREG)
Molecular weight	234.3
Vapour pressure, mmHg	0.0000002 20 °C (PESREG) 0.0000002 20 °C, Morestan * (PESREG) 0.0000004 25 °C (PESREG)
Water solubility, mg/l	1 at 20 °C (PESREG)

Fat solubility, g/100g	0.08 OECD (PESREG)
Melting point, °C	169.8–170.0 °C (PESREG)
Log octanol/water coefficient, log Pow	3.78 (PESREG)
Henry's law constant, Pa x m³/mol	0.00608 at 20 °C (PESREG)
Adsorption/desorption	Chinomethionat adsorption coefficients (Ka) determined by the Freundlich equation were 37 for sandy loam and 41 for silt loam. Desorption of (C-13, C-14) chinomethionat from soils was also studied and the desorption coefficient (Kd) were 45 for sandy loam and 74 for silt loam. (PESREG) Aqueous solutions of (C-14) chinomethionat were equilibrated with four soil types and the adsorption and desorption coefficients and constants were determined.

soil type	*% organic carbon*	*adsorption Ka*	*adsorption Koc*	*desorption Kd*	*desorption Koc*
sand	0.526	72	13608	865	164320
sandy loam	0.579	93	16047	889	153479
silt loam	1.53	143	9366	998	65354
clay loam	1.16	140	12100	1084	93595

(PESREG)

Adsorption cofficient	37 sandy loam (PESREG) 41 silt loam (PESREG)
Desorption cofficient	45 sandy loam (PESREG) 74 silt loam (PESREG)
Mobility	Rf-values of Morestan on soil thin-layer plates varies 0.04 –0.1 (six different soils). (PESREG) In soil column study (sandy loam soil, incubated 30 days, rainfall 45 days, 1.25 cm daily) 4% of the applied original radioactivity was found in the water passed through the soil columns. 90% was retained in the upper 1.25 cm. (PESREG) In the soil column studies chinomethionat (0.0255 kg/ha) wasn't found (analysis unit 0.0002 mg/l) in the leachate of three soil samples after two days rainfall (200 mm). (PESREG) The leaching behaviour of (C-14) chinomethionat was studied in the soil (standard soil and aged soil) columns. 0.6–0.7% of applied (C-14) chinomethionat was found in leachate water (400 ml/2d) of standard soil columns and 6.8–6.9% in leachate water (400 ml/4d) of aged soil columns. In studies on the metabolism of chinomethionat in the soil, QDOH was detected as the major metabolite. (PESREG) Dust-air mixture may be explosive, if there is dust over 200 g/m³. Non corrosive. (Morestan *) PESREG Sublimates above the melting point. PESREG Solubility in organic solvents (mg/100 ml) at 20 °C: n-hexane: 100–200 dichloromethane: 2000–5000 2-propanol: 10–100 toluene: 2000–5000 (PESREG)

Photochemical degradation in soil

Morestan was irradiated on soil using a high pressure mercury lamp. The half-life of Morestan was 14 days. Identified photolysis products were 2,9-dimethyl(1,4)dithiino-(2,3-b:5,6-b')diquinoxaline (dimer) and 6-methyl-1,4-dihydro-2,3-quinoxalinedione (QDOH). (PESREG)

A half-life of chinomethionat on silica gel plates at irradiation with sunlight-simulating influorescent tubes was 1.2 days. A half-life of 5.5 days was calculated for the non-irradiated samples. (PESREG)

The measured half-life for (C-14) chinomethionat on sterilized sandy loam (pH 6.9) under natural sunlight was 28 days; the net photolysis half-life was 49 days. The photolysis products were 6-methyl-2,3-dihydroxy-quinoxaline (QDOH) and 1,2,3,4-tetrahydro-2,3-dioxo-quinoxalinecarboxylic acid (Acid QDOH). (PESREG)

Photochemical degradation in water

In a irradiation test (high-pressure mercury lamp) half-life of chinomethionat solution was 33 minutes. (PESREG)

The photolysis (medium-pressure mercury vapour lamp) half-life of (C-14) Morestan in an aqueous buffer solution (pH 5) was 13.2 hours. The major photoproduct was 1,4-dihydro-6-methyl-2,3-quinoxalinedione (QDOH). (PESREG)

Hydrolysis in water

The hydrolysis half-life of Morestan in buffer solutions (0.8 ppm, 25 °C) was 2 hours (pH 9), 2 days (pH 7) and 7 days (pH 5). The major hydrolysis products were 1,4-dihydro-6-methyl-2,3-quinoxalinedione (QDOH) and 2,9- or 2,10-dimethyl(1,4)dithiino(2,3-b:5,6-b')diquinoxaline (dimer) (pH 9) and the dimer (pH 7 and 5). (PESREG)

The half-life of chinomethionat (pH 7):

conc. mg/l	*°C*	*half-life*
0.205	40	8hr
0.185	50	3hr
0.177	60	1hr
0.114	70	19 min.

(PESREG)

0.05 ppm of the technical chinomethionat in buffered solution (pH 7, 30 °C) gave half-life of 33 hours. (PESREG)

The half-life of chinomethionat (0.25 ppm) was 80 hours (pH 7, 22 °C) and the hydrolyse product was 1,4-dihydro-6-methyl-2,3-quinoxalinedithiol (QDSH). (PESREC)

Hydrolysis in acid

The half-life of chinomethionat (pH 4):

conc. mg/l	*°C*	*half-life*
0.205	50	19hr
0.212	60	8hr
0.209	70	4hr.

(PESREG)

0.05 ppm of the technical chinomethionat in buffered solution (pH 5, 30 °C) gave half-life of 109 hours. (PESREG)

The half-life of chinomethionat (0.25 ppm) was 240 hours (pH 4, 22 °C) and the hydrolyse product was 1,4-dihydro-6-methyl-2,3-quinoxalinedithiol (QDSH). (PESREG)

Hydrolysis in base

The half-life of chinomethionat (pH 9):

conc. mg/l	*°C*	*half-life*
0.168	20	5hr
0.212	30	1hr.

(PESREG)

The half-life of chinomethionat (0.25 ppm) was < 4 hours (pH 9, 22 °C) and the hydrolyse product was 1,4-dihydro-6-methyl-2,3-quinoxalinedithiol (QDSH). (PESREG)

Aerobic degradation in soil

The half-life of Morestan 25% WP (2.5 kg a.i./ha) under non-sterile aerobic conditions was 4 days in sandy loam and < 1 day in silt loam. Under sterile aerobic conditions the half-life of Morestan was 52 days in sandy loam and 18 days in silt loam. The major metabolite (QDOH) and four minor metabolites (QDSOH, QDSH, acid QDOH and dimer) were indentified in the soils. (PESREG)

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Degradation and transformation products	6-methyl-1,4-dihydro-2,3-quinoxalinedione (QDOH) 2-hydroxy or 3-hydroxy-6-methyl2(1H)quinoxalinethione (QDSOH) 6-methyl-1,4-dihydroxy-2,3-quinoxalinedithione (QDSH) 1,2,3,4-tetrahydro-2,3-dioxo-6-quinoxalinecarboxylic acid (acid QDOH) 2,9- or 2,10-dimethyl(1,4)dithiino(2,3-b:5,6-b')diquinoxaline (dimer). (PESREG)
Bioconcentration factor, fishes	78 56d, 0.05 ppm, whole body Cyprinus carpio 113 14d, 0.005 ppm, whole body Cyprinus carpio 1100 14d, 1 ppb, whole body Lepomis macrochirus (PESREG)
LD50 values to mammals in oral exposure, mg/kg	3009 orl-rat male, Morestan * (PESREG) 2424 orl-rat female, Morestan * (PESREG) 2272–3079 orl-rat male (PESREG) 2179–5190 orl-rat male, fed (PESREG) 1080–2275 orl-rat male, not fed (PESREG) 1513–2142 orl-rat male (PESREG) 917–1320 orl-rat female (PESREG) > 1000 orl-cat 1000< LD50< 2500 orl-rat male (PESREG)
LD50 values to mammals in non-oral exposure, mg/kg	> 1000, idr-rat, Morestan * (PESREG) > 5000 idr-rat, Morestan * (PESREG) > 2000 idr-rat (PESREG) > 1000 idr-rat (PESREG)
LC50 values to mammals in inhalation exposure, mg/m³	> 304 mg/m³, 4hr, ihl-rat, Morestan * > 4680 mg/m³, 4hr, ihl-rat male 2162 4hr, ihl-rat female (PESREG)
LC50 values to mammals in inhalation exposure, ppm	0.00005 > 0.05 ppb, 4hr, ihl-rbt (PESREG) 0.00005 > 0.05 ppb, 4hr, ihl-ham (PESREG) 0.00005 > 0.05 ppb, 4hr, ihl-rat (PESREG) 0.00005 > 0.05 ppb, 4hr, ihl-mus (PESREG) 0.00005 > 0.05 ppb, 4hr, ihl-cat (PESREG)
LD50 values to birds in oral exposure, mg/kg	196 14d, orl-brd, Colinus virginianus (PESREG)
Subacute LC50 values to birds in feeding exposure, mg/kg	> 5000 5d+3d, Anas platyrhynchos 2409 5d+3d, Colinus virginianus (PESREG)
NOEC values to birds in oral exposure, mg/kg	30 14d, orl-brd, Colinus virginialus (PESREG)
Effects on invertebrates	LC50, > 1000 mg/kg, 14d, Eisenia foetida, GLP, OECD No 207 LLC, > 1000 mg/kg, 14d, Eisenia foetida, GLP, OECD No 207 LOEC, 1000 mg/kg, 14d, Eisenia foetida, GLP, OECD No 207 NOEC, 100 mg/kg, 14d, Eisenia foetida, GLP, OECD No 207 Morestan * (PESREG) LC50, > 260 mg/kg, 14d, Eisenia foetida, GLP, OECD No 207 LLC, > 260 mg/kg, 14d, Eisenia foetida, GLP, OECD No 207 LOEC, 260 mg/kg, 14d, Eisenia foetida, GLP, OECD No 207 NOEC, 26 mg/kg, 14d, Eisenia foetida, GLP, OECD No 207 (PESREG)
Effects on bees	LD50, 0.06647 mg/bee, 48hr, at 26.7 °C, Morestan * (PESREG)

C

Effects on arthropods	Reduction of laying eggs 99%, conc. 0.1, Coccygomimus turionellae. No effect to mortality, Coelotes terrestris. (Albert et al. 1984)
Effects on microorganisms	Morestan 25 WP was used as aqueous solution. No inhibition of bacteria and actinomycetes was seen until Morestan exceeded 1000 ppm. Cellulomonas flavigena showed inhibition of growth at 10000 ppm Morestan. Morestan at 2 to 10 ppm caused 0 to 13% inhibition in growth of Aspergillus niger and Penicillium daleae and 11 to 63% inhibition in growth of Trichoderma viride and Phycomyces nitens. (PESREG)

Significant differences were recognized on soil respiration between chinomethionat treated and untreated soil:

soil	*mg chinomethionat /kg in soil*	*days after treatment*	*soil respiration significant difference carbon dioxide*
LOAMY SAND			
without lucerne-grass	3.3	14	+
	3.3	21	+
with lucerne-grass	3.3	14	+
SANDY SILT			
without lucerne-grass	0.33	21	+
	3.3	7	+
	3.3	21	+
with lucerne-grass	3.3	14	+

(PESREG)

Morestan WP 25 treatment (1 ppm, 30 °C, 4 days) didn't cause any significant effect on the asymbiotic nitrogen fixing microbes compared to controls in sandy loam. (PESREG)

A significant increase in nitrogen fixation was observed in soybeans grown in Morestan 25% WP treated (1.13 ppm a.i., 4 weeks) sandy loam soil compared to controls. (PESREG)

The nitrification of Morestan 25 WP treated (0.5 ppm or 5 ppm a.i., 30 °C, 7, 21 or 35 days) sandy loam soil samples differed from controls by a maximum of 1%. The denitrification samples varied by 1% or less from the control samples. (PESREG)

Significant differences in mineralization of nitrogen were observed between chinomethionat treated and control soil samples:

soil	*mg chinomethionat a.i./kg soil*	*days after in treatment*	*significant difference ammonium*	*nitrat*
loamy sand	0.33	0	+	
	0.33	14	+	
sandy silt	0.33	7	+	
	0.33	21	+	+
	0.33	28		+
	3.3	7	+	
	3.3	14	+	
	3.3	28		+
loamy sand after	0.33	21	+	
amendment with ammonium	3.3	28		+

(PESREG)

EC50 values to algae, mg/l	0.049 0.056 0.22 0.24	72hr, grw bms, Scenedesmus subspicatus 96hr, grw bms, Scenedesmus subspicatus 72hr, grw rate, Scenedesmus subspicatus 96hr, grw rate, Scenedesmus subspicatus Morestan *, GLP, ISO/DIS 8692, OECD 201 (PESREG)
	0.064 0.068 0.1 0.14	72hr, grw bms, Scenedesmus subspicatus 96hr, grw bms, Scenedesmus subspicatus 72hr, grw rate, Scenedesmus subspicatus 96hr, grw rate, Scenedesmus subspicatus GLP, ISO/DIS 8692, OECD No 201 (PESREG)
LOEC values to algae, mg/l	0.032	96hr, Scenedesmus subspicatus Morestan *, GLP, ISO/DIS 8692, OECD 201 (PESREG)
	0.056	96hr, Scenedesmus subspicatus GLP, ISO/DIS 8692, OECD No 201 (PESREG)
NOEC values to algae, mg/l	0.01	96hr, Scenedesmus subspicatus Morestan *, GLP, ISO/DIS 8692, OECD 201 (PESREG)
	0.032	96hr, Scenedesmus subspicatus GLP, ISO/DIS 8692, OECD No 201 (PESREG)
EC50 values to crustaceans, mg/l	0.12	48hr, act imb, Daphnia magna (OECD 202, PESREG)
LOEC values to crustaceans, mg/l	> 0.018 0.018	21d, rpd, Daphnia magna 21d, grw, Daphnia magna GLP, OECD 202 (PESREG)
	0.0223 0.00456	21d, rpd, Daphnia magna 21d, grw, Daphnia magna GLP, OECD 202 (PESREG)
NOEC values to crustaceans, mg/l	> 0.018 0.01	21d, rpd, Daphnia magna 21d, grw, Daphnia magna GLP, OECD 202 (PESREG)
	0.0109 0.00245	21d, rpd, Daphnia magna 21d, grw, Daphnia magna GLP, OECD 202 (PESREG)
LC50 values to fishes, mg/l	1.03 0.94	96hr, Salmo gairdneri 96hr, Leuciscus idus melanotus Morestan * (PESREG)
	0.23–0.25 0.20–0.28 0.22 0.12	96hr, Leuciscus idus melanotus 96hr, Salmo gairdneri 96hr, Salmo gairdneri 96hr, Lepomis machrochirus (PESREG)

440 • Chloramine

127-65-1

LC50 values to crustaceans, mg/l	0.22	96hr, Gammarus pseudolimnaeus (Kemp et al. 1973)
LC50 values to fishes, mg/l	0.15	72hr, Pimephales promelas (Kemp et al. 1973)

441 • Chlordane

57-74-9

Synonyms	1,2,4,5,6,7,8,8-Octachloro-3a,4,7,7a-tetrahydro-4,7-endomethano-indene 1,2,4,5,6,7,8,8-Octachloro-4,7-methano-3a,4,7,7a-tetrahydro-indane	
Products containing the chemical	CD-68 Velsicol 1068 Toxichlor Niran Octachlor Ortho-klor Synklor Corodane Belt	
Use	Insecticide, fungicide.	
State and appearance	Colourless to amber. Viscous liquid.	
Odour	Odourless. Threshold odour concentration in water: 2.5 ppb; detection: 0.5 ppb (Verschueren 1983, Sigworth 1964).	
Molecular weight	409.76	
Water solubility, mg/l	0.009	technical chlordane
Log octanol/water coefficient, log Pow	6	(Mackay 1982)
Half-life in soil, days	3500	(Li et al. 1990)
Total degradation in soil	75–100% disappearance from soils: 3–5 years (Verschueren 1983).	
Other information about degradation	Persistence in river water in a sealed glass jar under sunlight and artificial fluorescent light – initial concentration 0.010 mg/l: *% of original compound found* after 1hr 1wk 2wk 4wk 8wk 100 90 85 85 85 (Eichelberger & Lichtenberg 1971).	
Bioconcentration factor, fishes	322 990	Lepomis macrochirus, cis-chlordane Carassius auratus, cis-chlordane (Khan et al. 1979)
Bioconcentration factor, mollusca	7300	oyster (Verschueren 1983)
Bioconcentration factor, algae	98000	Oedogonium, filamentous green alga 14C-cis:trans (75:25) chlordane (Verschueren 1983)
	6000 15000	6000- 15000, Scenedesmus cis(α- trans(γ)chlordane (Glooschenko et al. 1979)
Bioconcentration factor, other organisms	108	Xenopus laevis, 5 ppb cis-chlordane (Khan et al. 1979)
Other information about bioaccumulation	Confirmed to be accumulated on a high level (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	283 100	orl-rat orl-rbt (Lewis & Sweet 1984)
	457–590	orl-rat (Martin 1968)

LD50 values to mammals in non-oral exposure, mg/kg	690 skn-rat (Lewis & Sweet 1984) 457–590 ukn-rat (Virtanen & Nuuja 1987)
LDLo values to mammals in oral exposure, mg/kg	40 orl-hmn (Lewis & Sweet 1984)
Effects on the physiology of mammals	In diet: rats fed for 104 weeks on a diet containing 15 ppm γ-chlordane suffered no higher mortality than the controls but histopathological changes in the liver were apparent (Martin 1968).
Health effects	Lethal dose to human 86–860 mg/kg (Virtanen & Nuuja 1987).
Carcinogenicity	NCI carcinogenesis bioassay completed: results positive, mus; results negative, rat (Lewis & Sweet 1984).
LD50 values to birds in oral exposure, mg/kg	220 orl-ckn 1200 orl-dck (Lewis & Sweet 1984)
Effects on arthropods	Pteronarcys californica: 96hr, Lc50: 0.015 mg/l (Sanders & Cope 1968). LC50, 1.440 mg/l, 48hr, static, Tanytarsus dissimilis (Holcombe et al. 1983).
Effects on microorganisms	Bacteria: oral Viridans streptococci: total inhibition at 3.0 ppm (Goes et al. 1978).
LC50 values to crustaceans, mg/l	0.0004 96hr, Penaeus duorarum 0.0062 Crassostrea virginia 0.0048 Palaemonetes pugio (Parrish et al. 1976) 0.026 96hr, Gammarus lacustris (Sanders 1969) 0.04 96hr, Gammarus fasciatus 0.004 96hr, Palaemonetes kadiakensis 0.0025 120hr, Palaemonetes kadiakensis (Sanders 1972) 0.02 48hr, Simocephalus serrulatus 0.029 48hr, Daphnia pulex (Sanders & Cope 1966) 0.00042 96hr, Saccobranchus fossilis (Verma et al. 1978) 0.59 48hr, Daphnia (Pesticide Manual 1983) 0.029 act, Daphnia magna (Kenaga 1979)
EC50 values to crustaceans, mg/l	0.029 48hr, Daphnia pulex (Shapiro 1979) 0.097 technical chlorinated chlordane 0.813 techn. dechlorinated chlordane 0.156 72% emulsifiable concentrate, chlorinated 1.174 72% emul.concentrate, dechlorinated 48hr, Daphnia (Randall et al. 1979)

LC50 values to fishes, mg/l	0.008	96hr, Salmo gairdneri
	0.069	act, Pimephales promelas (Kenaga 1979)
	0.09	96hr, Salmo gairdneri (Pesticide Manual 1983)
	0.341	96hr, Poecilia reticulata (Gupta et al. 1984)
	0.037	96hr, Pimephales promelas
	0.047	96hr, Salvelinus fontinalis
	0.059	96hr, Lepomis macrochirus (Cardwell et al. 1977)
	0.041	technical chlorinated chlordane
	0.582	techn. dechlorinated chlordane
	0.062	72% emulsifiable concentrate, chlorinated
	0.8	72% emul.concentrate, dechlorinated 96hr, Lepomis macrochirus (Randall et al. 1979)
	Technical chlordane consist of 60 to 75% isomers of chlordane and 25 to 40% of related compounds including 2 isomers of heptachlor and one each of enneachloro- and decachlorodicyclopentadiene Two isomers of octachlorodicyclopentadiene have been isolated from chlordane of which α-chlordane is the endo-cis anβ-chlordane is the endo-trans isomer. The commercial product known as γ-chlordane is substantially th α-isomer. Technical chlordane is a mixture of 26 organochlorine compounds.	
	0.0064	96hr, Lagodon rhomboides
	0.0245	96hr, Cyprinodon variegarus (Parrish et al. 1976)
	0.0125	96hr, Cyprinodon variegarus (Parrish et al. 1978)
	0.42	96hr, Saccobranchus fossilis (Verma et al. 1978)
LOEC values to fishes, mg/l	0.018	srv, chr, Cyprinodon variegatus (Ward & Parrish 1980)
	0.0008	srv, chr, Cyprinodon variegatus (Parrish et al. 1978)
	0.0012	srv, chr, Lepomis macrochirus
	0.0003	srv, rpd, chr, Salvelinus fontinalis (Cardwell et al. 1977)
NOEC values to fishes, mg/l	0.0005	srv, chr, Cyprinodon variegatus (Parrish et al. 1978)
	0.0005	srv, chr, Lepomis macrochirus (Cardwell et al. 1977)
Other information about water organisms	EC50 (24hr), 0.6 mg/l, rpd, Tetrahymena pyriformis (Yoshioka et al. 1985). 0.0001–0.1 mg/l, stimulation of growth, Scenedesmus quadricauda (Verschueren 1983). Chlamydomonas sp. (soil alga): 0.0001–0.050 mg/l, stimulation of growth 0.100 mg/l inhibition of cell division (Verschueren 1983). LC50, 1.25 mg/l, 96hr, static, Aplexa hypnorum (Holcombe et al. 1983).	

Other information	Approximate composition of technical chlordane: cis(α)chlordane (C10H6Cl8) * 19% trans(γ)chlordane (C10H6Cl8) * 24% chlordene (4 isomers) (C10H6Cl6) * 21.5% heptachlor (C10H5Cl7) * 10% nonachlor (C10H5Cl9) * 7% (C10H7-8Cl6-7) * 8.5% hexachlorocyclopentadiene (C5Cl6) * > 1% octachlorocyclopentadiene (C5Cl8) * 1% Diels-Alder adduct of cyclopentadiene and pentachlorocyclopentadiene (C10H6Cl5) * 2% others * 6% (Verschueren 1983).	

442 • Chlordene 3734-48-3

Use	Intermediate in the manufacturing of chlordane.
Effects on arthropods	Mosquito (late 3rd instar Aedes aegypti larvae) 24hr LC50: 130 ppb; housefly (3 day old female Musca) LD50: 0.158 mg/fly (Khan et al. 1973).
Other information about water organisms	Lepomis macrochirus; 24hr, LC50: 218 ppb (Khan et al. 1973).

443 • Chlorfenson 80-33-1

Synonyms	4-Chlorophenyl-4-chlorobenzenesulfonate	
Use	Acaricide.	
LC50 values to crustaceans, mg/l	> 10	act, Daphnia pulex (Nishiuchi & Hashimoto 1967)
LC50 values to fishes, mg/l	3.2	48hr, Cyprinus carpio (Pesticide Manual 1983)
	1.1	48hr, Cyprinus carpio (Nishiuchi & Hashimoto 1967)

444 • Chlorfenvinphos 470-90-6

Synonyms	2-Chloro-1-(2,4-dichlorophenyl)-vinyldiethylphosphate 0,0-Diethyl-0-1-(2',4'-dichlorophenyl)-2-chlorovinylphosphate	
Use	Insecticide.	
State and appearance	Amber coloured liquid.	
Molecular weight	359.58	
Specific gravity (water=1)	1.36	at 15.5/15.5 °C
Vapour pressure, mmHg	0.00000017 mmHg	
Melting point, °C	-16/-22	
Boiling point, °C	168–170 at 0.5 mm	
Log soil sorption coefficient, log Kom	2.23	(Sabljic 1987)

Total degradation in soil	Persistence in soil at 10 ppm initial concentration: *weeks incubation to* — *50% remaining* / *5% remaining* sterile sandy loam: > 24 sterile organic soil: > 24 non-sterile sandy loam: < 1 / 5 non-sterile organic soil: 1 / 9 (Miles et al. 1979).
LD50 values to mammals in oral exposure, mg/kg	10 orl-rat 20 orl-ctl (Lewis & Sweet 1984) > 12000 orl-dog 280–400 orl-rbt 117–200 orl-mus 10–39 orl-rat (Martin 1968)
LD50 values to mammals in non-oral exposure, mg/kg	26.4 skn-rat 400 skn-rbt (Lewis & Sweet 1984) 3200–4700 skn-rbt (Anon. 1976) 31–108 (Martin 1968)
TDLo values to mammals in non-oral exposure, mg/kg	10 skn-hmn (Lewis & Sweet 1984)
Other information about mammals	In diet: 90 days feeding tests with rats showed that diets containing up to 300 ppm had no adverse effects on growth or food consumption (Martin 1968).
LD50 values to birds in oral exposure, mg/kg	29 orl-ckn (Lewis & Sweet 1984) 10.0–13.3 orl-Agelaius phoeniceus 3.16–23.7 orl-Sturnus vulgaris 17.8–178 orl-Coturnix coturnix 13.3 orl-Passer domesticus 17.8 orl-Quiscalus quiscula 13.3 orl-Columba livia 23.7 orl-Carbodacus mexicanus 13.3 orl-Molothrus ater 178 orl-Zonotrichia atricapilla (Schafer et al. 1983)
LC50 values to crustaceans, mg/l	0.011 Daphnia pulex (Nishiuchi & Hashimoto 1976) 0.28 48hr, Daphnia magna 0.1 24hr, Daphnia magna (Bogacka & Groba 1980)
LC50 values to fishes, mg/l	0.27 48hr, Cyprinus carpio (Nishiuchi & Hashimoto 1967) 0.54 24hr, Poecilia reticulata (Pesticide Manual 1983) 1.78 48hr, Lebistes reticulatus 1.5 96hr, Lebistes reticulatus (Bogacka & Groba 1980)

445 • Chlorinated paraffines 63449-39-8

Products containing the chemical	Cereclor 42 * 48, 50LV etc. Chlorowax LV * 40 500 C etc. Chlorez 700 Witaclor 340 * etc.

Molecular weight	320; 1100
Density, kg/m³	1160 1160-1540, 25 °C (Zitko 1980)
Vapour pressure, mmHg	0.00002 20 °C (Howard et al. 1975)
Water solubility, mg/l	0.001 (Johansson 1982)
Log octanol/water coefficient, log Pow	4.4–12.8 (Renberg et al. 1980)
Other physicochemical properties	In fire PCB are formed, propably also chlorinated dibenzodioxins and dibenzofurans (Anon. 1989).
Photochemical degradation in air	No photochemical degradation in UV-light (290 nm) (Lombardo 1975).
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Other information about degradation	Paraffines with little chloride degrade aerobically (Madeley & Birtley 1980). Degradation decreases strongly when chain length and chlorination grade increases. For example CP (C10-13) with 50% Cl is degraded after adaption in 25 days (Madeley & Birtley 1980).
Bioconcentration factor, fishes	700–800 Witaclor 149, Witaclor 159 (Bengtsson & Baumann-Ofstad 1982)
Bioconcentration factor, mollusca	6000 Mytilus edulis (Johansson 1982)
Bioconcentration factor, other organisms	1000 aquatic organisms (Cambell & McConell 1980)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987). Short chained clorinated paraffines with high chlorination grade are most bioaccumulative (Bengtsson & Baumann-Ofstad 1982). No remarkable biomagnification in food chains of aquatic organisms (Svanberg 1983).
LD50 values to mammals in oral exposure, mg/kg	21850 orl-rat (Howard et al. 1975) 4000 orl-rat (Birtley et al. 1980)
Effects on the physiology of mammals	Weight increase in liver and changes in liver cells and in their subcellular structure in mammals (Birtley et al. 1980). Increase of cytochrom P-450 in liver and changes in enzyme activity (Birtley et al. 1980).
Carcinogenicity	No carcinogenic effects have been indicated (Svanberg 1983).
Mutagenicity	No mutagenic effects have been indicated (Svanberg 1983).
Other information about birds	No mortality, Cereflor S 52: suck, 10 300 mg/l; pheasant 24 600 mg/l (Madeley & Birtley 1980).
LC50 values to crustaceans, mg/l	0.06 96hr, Nitocra spinipes Witaclor 149, C10-13,49% Cl 0.1–10 000 Ceroclor, 5 products (Tarkpea et al. 1981)
LC50 values to fishes, mg/l	300 96hr, Salmo gairdneri Chlorowax, 5 products (Howard et al.1975) 520–1630 Cereclor 42 (Madeley & Birtley 1980) 300 96hr, Lepomis macrochirus Chlorowax,5 products (Howard et al.1975) 5000–10000 96hr, Alburnus alburnus, chlorinated paraffines (Linden et al.1979)

Effects on the physiology of water organisms	Neurotoxic effects, Alburnus alburnus, 14 days, Witachlor, 5 products, 0.125 mg/l (Svanberg 1983). Effects on mobility, Salmo gairdneri, 15–20 days, Chlorowax, 0.05 mg/l (Howard et al. 1975).
Effects on the reproduction of water organisms	Effects on reproduction, Platichtys flesus, 4 weeks, Witachlor 149, 2 products, 1 mg/l (Haux et al. 1982).
Other information	Organotin compounds which are used as stabilizers in CP can have an effect on toxicity of tested products (IMO 1989).

446 • Chlorinated paraffins (C = 20–22)

61788-76-9

Sumformula of the chemical	CnH2n+2-xClx
Water solubility, mg/l	< 100 (MITI 1992)
Melting point, °C	< -10 (MITI 1992)
Total degradation in water	Biodegradation: 3–6% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 1.0–4.9 6w, Cyprinus carpio, conc 2 mg/l < 10 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 250 48hr, Oryzias latipes (MITI 1992)

447 • Chlorine

7782-50-5

Sumformula of the chemical	Cl2
Use	Bleaching, desinfection.
Molecular weight	70.9
LC50 values to mammals in inhalation exposure, ppm	293 0.865 mg/l, 1hr, ihl-rat 137 1hr, ihl-mus (Lewis & Sweet 1984)
LCLo values to mammals in inhalation exposure, mg/kg	2530 ihl-hmn, 30min (Sweet 1987)
LCLo values to mammals in inhalation exposure, ppm	873 30 min, ihl-hmn (Lewis & Sweet 1984) ihl-cat, 4hr (Sweet 1987) ihl-dog, 30min ihl-gpg, 7hr ihl-hmn, 5min ihl-mam, 5min ihl-rbt, 4hr 30 min, ihl-hmn (Lewis & Sweet 1984) ihl-cat, 4hr (Sweet 1987) ihl-dog, 30min ihl-gpg, 7hr ihl-hmn, 5min ihl-mam, 5min ihl-rbt, 4hr

C

	660	30 min, ihl-hmn (Lewis & Sweet 1984) ihl-cat, 4hr (Sweet 1987) ihl-dog, 30min ihl-gpg, 7hr ihl-hmn, 5min ihl-mam, 5min ihl-rbt, 4hr
	800	30 min, ihl-hmn (Lewis & Sweet 1984) ihl-cat, 4hr (Sweet 1987) ihl-dog, 30min ihl-gpg, 7hr ihl-hmn, 5min ihl-mam, 5min ihl-rbt, 4hr
	330	30 min, ihl-hmn (Lewis & Sweet 1984) ihl-cat, 4hr (Sweet 1987) ihl-dog, 30min ihl-gpg, 7hr ihl-hmn, 5min ihl-mam, 5min ihl-rbt, 4hr
	500	30 min, ihl-hmn (Lewis & Sweet 1984) ihl-cat, 4hr (Sweet 1987) ihl-dog, 30minihl-gpg, 7h rihl-hmn, 5min ihl-mam, 5min ihl-rbt, 4hr
	500	30 min, ihl-hmn (Lewis & Sweet 1984) ihl-cat, 4hr (Sweet 1987) ihl-dog, 30min ihl-gpg, 7hr ihl-hmn, 5min ihl-mam, 5min ihl-rbt, 4hr
	660	30 min, ihl-hmn (Lewis & Sweet 1984) ihl-cat, 4hr (Sweet 1987) ihl-dog, 30min ihl-gpg, 7hr ihl-hmn, 5min ihl-mam, 5min ihl-rbt, 4hr
Mutagenicity	Mutation data: cyt, hmn, lym, 20 ppm; sperm morphology, mus, orl, 20 mg/kg (Sweet 1987).	
Effects on plants	It is recommended that Cl applied as chlorine containing fertilizer (to tobacco, Nicotiana tabacum) should not exceed 4 kg Cl/10 a. Excessive application of Cl causes definite damage (Ishizaki & Akiya 1978).	
NOEC values to crustaceans, mg/l	0.003	rpd, schr, Daphnia magna (Arthur 1971)

LC50 values to fishes, mg/l	0.014	96hr, Salmo gairdneri (Leach & Thakore 1975)
	0.5	96hr, Gambusia affinis (Cohen & Valenzuela 1977)
	2.1	96hr, Salmo gairdneri (Voss et al. 1980)
	0.84	1hr, Gambusia affinis (Mattice et al. 1981)
	0.068	96hr, Salvelinus fontinalis (Ward & DeGraeve 1980)
	0.037	96hr, Salmo gairdneri (Ward & DeGraeve 1980)
	0.12	96hr, Pimephales promelas (Ward & DeGraeve 1980)
	0.09–0.11	96hr, Salmo trutta m. lacustris (Larson et al. 1978)
	0.053–0.083	96hr, Salmo trutta m. lacustris (Larson et al. 1978)
LOEC values to fishes, mg/l	0.042	srv, schr, Pimephales promelas (Arthur et al. 1975)
NOEC values to fishes, mg/l	0.014	srv, schr, Pimephales promelas (Arthur et al. 1975)

C

448 • Chlormephos 24934-91-6

Synonyms	S-Chloromethyl-0,0-diethylphosphorothiolothionate	
Use	Insecticide.	
Specific gravity (water=1)	1.26	
LD50 values to mammals in oral exposure, mg/kg	7	orl-rat (Verschueren 1983)
LD50 values to mammals in non-oral exposure, mg/kg	27	skn-rat (Verschueren 1983)
LC50 values to fishes, mg/l	2.5	96hr, Rasbora heteromorpha (Tooby et al. 1975)

449 • Chlormequat 999-81-5

Synonyms	(2-Chloroethyl) trimethylammonium chloride CCC	
LD50 values to mammals in oral exposure, mg/kg	54 20	orl-mus orl-cat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	232	skn-rbt (Lewis & Sweet 1984)
LDLo values to mammals in oral exposure, mg/kg	10	orl-hmn (Lewis & Sweet 1984)
Carcinogenicity	NCI carcinogenesis bioassay completed: results negative; mus, rat (Lewis & Sweet 1984).	
Effects on plants	Cultivars of wheat (Triticum aestivum), barley (Hordeum vulgare) and oats (Avena sativa) were sprayed at the 3- to 5-leaf stage with an aqueous solution of CCC at a concentration -1 of 10 M → heights of the cereals were reduced, foliage of the three crops showed symptoms of toxicity in the form of extensive bleached whitish areas in the leaves. (Clark & Fedak 1977)	

450 • Chloro(2-methoxyethyl)mercury 123-88-6

Synonyms	Agallol Aratan Baytan Emisan 6 Falisan Gramisan Higosan Triadimenol Tafasan
Sumformula of the chemical	C3H7ClHgO
Use	Fungicide.
Molecular weight	295.14
LD50 values to mammals in oral exposure, mg/kg	22 orl-rat 47 orl-mus (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	60 scu-mus (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	> 316 orl-Agelaius phoeniceus (Schafer et al. 1983)
LC50 values to fishes, mg/l	0.91 96hr, Gambusia affinis (Joshi & Rege 1980) 0.205–0.445 96hr, Cyprinus carpio (Das et al. 1980)
Effects on the physiology of water organisms	Channa punctatus; 20 mg/l; 180d, biochemical effect (change in physiochemical process including glycogen uptake, cholesterol levels and lipid analysis) (Ram & Sathyanesan 1987).

451 • 4-Chloro-α,α,α-trifluorotoluene 98-56-6

Sumformula of the chemical	C7H4ClF3
EC50 values to microorganism, mg/l	11.4 Microtox (Kaiser et al. 1985)

452 • 2-Chloro-1-(2,4,5-trichlorophenyl) vinyl dimethylphosphate 961-11-5

Sumformula of the chemical	C10H9Cl4O4P
Water solubility, mg/l	14 (MITI 1992)
Melting point, °C	97–98 (MITI 1992)
Log octanol/water coefficient, log Pow	3.57 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

Bioconcentration factor, fishes	37–62 28–52	8w, Cyprinus carpio, conc 0.05 mg/l 8w, Cyprinus carpio, conc 0.005 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	7.46	48hr, Oryzias latipes (MITI 1992)

453 • 3-Chloro-1,2-propanediol 96-24-2

Synonyms	3-Chloro-1,2-propylene glycol	
Boiling point, °C	139	18 mmHg (MITI 1992)
Chemical oxygen demand, g 02/g	0.98	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.01	5 days (Bridie et al. 1979)
Total degradation in water	Biodegradation: 68% by BOD period: 14d substance: 100 mg/l sludge: 30mg/l (MITI 1992).	
LD50 values to birds in oral exposure, mg/kg	23.7 316–422	orl-Agelaius phoeniceus orl-Coturnix coturnix (Schafer et al. 1983)
LC50 values to fishes, mg/l	> 5000	Carassius auratus (Bridie et al. 1979)

454 • 4-Chloro-1-nitro-2-(trifluoro-methyl)benzene 118-83-2

Sumformula of the chemical	C7H3ClF3NO2	
EINECS-number	2042807	
Water solubility, mg/l	100	(MITI 1992)
Melting point, °C	21	(MITI 1992)
Log octanol/water coefficient, log Pow	3.2	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance:100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	43–141 28–120	8w, Cyprinus carpio, conc 0.01 mg/l 8w, Cyprinus carpio, conc 0.001 mg/l (MITI 1992)
LC50 values to fishes, mg/l	15.3	48hr, Oryzias latipes (MITI 1992)

455 • 1-Chloro-1-nitropropane 16984-48-8

Sumformula of the chemical	C2H5CH(NO2)Cl	
Molecular weight	123.5	
Vapour density (air=1)	4.26	
Conversion factor, 1 ppm in air=	5.05	
Conversion factor, 1 mg/m³ in air=	0.198	
Vapour pressure, mmHg	5.8	25 °C
Water solubility, mg/l	6	20 °C
Boiling point, °C	139–143 °C	
Other information about mammals	Rabbit: oral lethal dose: 0.05–0.10 g/kg	

456 • 3-Chloro-1-propanol 627-30-5

Chemical oxygen demand, g 02/g	1.36	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.06	5 days (Bridie et al. 1979)
LC50 values to fishes, mg/l	50	96hr, Carassius auratus (Bridie et al. 1979)

457 • 1-Chloro-2-(1,2-epoxyethyl)-benzene 2142-68-9

Sumformula of the chemical	C8H7ClO	
Boiling point, °C	180	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

458 • 1-Chloro-2-(1,2-ethane-diol)-benzene 59365-6-5

Sumformula of the chemical	C8H9Cl	
Log octanol/water coefficient, log Pow	1.17	(MITI 1992)
Bioconcentration factor, fishes	1.1–1.3 < 3.5	6w, Cyprinus carpio, conc 1 mg/l 6w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 500	48hr, Oryzias latipes (MITI 1992)

459 • 5-Chloro-2-(2,4-dichloro-phenoxy) phenol

3380-34-5

Synonyms	2,4,4'-Trichloro-2'-hydroxydiphenyl ether
Water solubility, mg/l	17 (MITI 1992)
Melting point, °C	55–57 (MITI 1992)
Log octanol/water coefficient, log Pow	4.76 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	2.7–44 8w, Cyprinus carpio, conc 0.03 mg/l 15–90 8w, Cyprinus carpio, conc 0.003 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	2.04 48hr, Oryzias latipes (MITI 1992)

460 • 1-Chloro-2,4-dinitrobenzene

97-00-7

LC50 values to fishes, mg/l	0.12 14 d, Poecilia reticulata (Hermens et al. 1984)

461 • 5-Chloro-2-methyl-4-isotiazoline-3-one

26172-55-4

Use	Slimicide.
LC50 values to fishes, mg/l	6.1 96hr, Branchydanio rerio (Björndal et al. 1984)
LOEC values to fishes, mg/l	2 srv, schr, Branchydanio rerio (Björndal et al. 1984)

462 • 4-Chloro-2-methylaniline

95-69-2

Synonyms	4-Chloro-o-toluidine 2-Amino-5-chlorotoluene Azogene FastRed TR 5-Chloro-2-aminotoluene 4-Chloro-2-methylbenzeneamine 4-Chloro-2-toluidine 4-Chloro-6-methylaniline Deval Red TR 2-Methyl-4-chloroaniline Red Base NTR Chloromethylaniline
Sumformula of the chemical	C7H8ClN
Molecular weight	141.61
Melting point, °C	> 26.8 (MITI 1992)

Boiling point, °C	240	760 mmHg (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	7.7–12.0 < 35	6w, Cyprinus carpio, conc 0.34 mg/l 6w, Cyprinus carpio, conc 0.034 mg/l (MITI 1992)
LDLo values to mammals in non-oral exposure, mg/kg	310	scu-cat (Sweet 1987)
LD50 values to birds in oral exposure, mg/kg	75 75 > 100	orl-wild bird (Sweet 1987) orl-Agelaius phoeniceus Sturus vulgaris (Schafer et al. 1983)
LC50 values to fishes, mg/l	34	48hr, Oryzias latipes (MITI 1992)
Other information	Biodegradation product of chlorphenamidine (Verschueren 1983).	

463 • 4-Chloro-2-nitroaniline 89-63-4

Melting point, °C	116–117.6	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).	
Bioconcentration factor, fishes	7.5–13.2 8.0–13.4	6w, Cyprinus carpio, conc 0.1 mg/l 6w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	17.4	48hr, Oryzias latipes (MITI 1992)

464 • 5-Chloro-2-nitrotoluene 5367-28-2

EC50 values to microorganism, mg/l	8.91 8.05	15 min, Photobacterium phosphoreum 30 min, Photobacterium phosphoreum (Anon. 1986b)

465 • 1-Chloro-3-bromopropane 109-70-6

Synonyms	3-Bromopropyl chloride 1-Bromo-3-chloropropane 3-Chloropropyl bromide Trimethylenebromide chloride Trimethylene chlorobromide

Sumformula of the chemical	C3H6BrCl	
Molecular weight	157.45	
Other physicochemical properties	Moderately toxic by ingestion. When heated to decomposition it emits toxic fumes of Cl- and Br-.	
Chemical oxygen demand, g 02/g	0.84	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.02	5 days (Bridie et al. 1979)
LD50 values to mammals in oral exposure, mg/kg	930 1290	orl-rat orl-mus (Sax & Lewis 1989)
LC50 values to mammals in inhalation exposure, mg/m³	5668	ihl-rat (Sax & Lewis 1989)
LCLo values to mammals in inhalation exposure, mg/kg	7270	2hr, ihl-mus (Sax & Lewis 1989)
LC50 values to fishes, mg/l	75	24hr, Carassius auratus (Bridie et al. 1979)

466 • 6-Chloro-3-cresol 615-74-7

Synonyms	6-Chloro-m-cresol	
Water solubility, mg/l	> 1000	(MITI 1992)
Total degradation in water	Biodegradation: 0–11% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	1.2–4.7 < 2.7–4.0	6w, Cyprinus carpio, conc 0.02 mg/l 6w, Cyprinus carpio, conc 0.002 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LD50 values to birds in oral exposure, mg/kg	562 750 562 562	orl-Agelaius phoeniceus orl-Sturnus vulgaris orl-Coturnix coturnix orl-Passer domesticus (Schafer et al. 1983)
LC50 values to fishes, mg/l	5.6	48hr, Oryzias latipes (MITI 1992)

467 • 4-Chloro-3-methylphenol 59-50-7

Synonyms	p-Chloro-m-cresol 6-Chloro-3-hydroxytoluene 4-Chloro-3-hydroxytoluene PCMC 4-Chloro-1-hydroxy-3-methylbenzene 3-Methyl-4-chlorophenol; 4-Chloro-3-cresol p-Chlorocresol
Sumformula of the chemical	C7H7ClO

Use	External germicide; preservative for glues, glums, inks, textile and leather goods.	
State and appearance	Odourless crystals (when pure).	
Odour	Odourless when pure. In water: odour threshold; 0.1 mg/kg (Verschueren 1983).	
Molecular weight	142.6	
Water solubility, mg/l	> 1000	(MITI 1992)
Melting point, °C	64–66	(MITI 1992)
Boiling point, °C	235	
Log octanol/water coefficient, log Pow	3.1	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28w substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	6.7–13 5.5–11	6w, Cyprinus carpio, conc 0.02 mg/l 6w, Cyprinus carpio, conc 0.002 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	1830	orl-rat (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	400	scu-rat (Sweet 1987)
LDLo values to mammals in non-oral exposure, mg/kg	200 30	scu-mus ipr-mus (Sweet 1987)
LD50 values to birds in oral exposure, mg/kg	≥ 113	orl-Agelaius phoeniceus (Schafer et al. 1983)
LC50 values to fishes, mg/l	7.6 4.6	96hr, Pimephales promelas (Holcombe et al. 1984) 48hr, Oryzias latipes (MITI 1992)
Other information about water organisms	Tetrahymena pyriformis, EC50, grw, 2 d, 22.86 mg/l (Schultz 1987).	

468 • 1-Chloro-3-nitrobenzene 121-73-3

Synonyms	m-Nitrochlorobenzene Chloro-m-nitrobenzene m-Chloronitrobenzene 3-Chloronitrobenzene	
Sumformula of the chemical	$C6H4ClNO2$	
Use	Manufacturing dyestuffs; intermediate in organic chemicals synthesis.	
State and appearance	Pale yellow chrystals.	
Odour	Odour threshold: 0,02 mg/m³	
Molecular weight	157.56	
Specific gravity (water=1)	1.534	20/4 °C

Melting point, °C	23.7 44.4	unst. stab.
Boiling point, °C	235–236	
Log octanol/water coefficient, log Pow	2.41 2.46	
Other information about degradation	Biodegradation: decomposition period by a soil microflora: > 64 days	
LD50 values to mammals in oral exposure, mg/kg	390	orl-mus (Lewis & Sweet 1983)
TCLo values to mammals in inhalation exposure, mg/kg	0.012	ihl-hmn (Lewis & Sweet 1983)
EC50 values to microorganism, mg/l	15.7	Microtox (Kaiser and Ribo 1985)
LC50 values to fishes, mg/l	1.2 18	96hr, Lepomis macrochirus (Dawson et al. 1977a) 96hr, Pimephales promelas (Holcombe et al. 1984)

469 • 1-Chloro-4-fluorobenzene 352-33-0

EC50 values to microorganism, mg/l	98.6	Microtox (Kaiser et al. 1985)

470 • 1-Chloro-4-iodobenzene 637-87-6

EC50 values to microorganism, mg/l	2.2	Microtox (Kaiser et al. 1985)

471 • 2-Chloro-4-nitrotoluene 121-86-8

Synonyms	Benzene, 2-chloro-1-methyl-4-nitro-	
Sumformula of the chemical	C7H6ClNO2	
EINECS–number	2045017	
EC50 values to microorganism, mg/l	13.5 14.5	15 min, Photobacterium phosphoreum 30 min, Photobacterium phosphoreum (Anon. 1986b)
EC50 values to crustaceans, mg/l	4	24hr, Daphnia magna (AQUIRE 1994)

472 • 2-Chloro-6-(trichloromethyl)-pyridine 1929-82-4

Synonyms	Nitrapyrin Dowco 163 N-serve N-serve nitrogen stabilizer
Sumformula of the chemical	C6H3Cl4N
Chemicals in the product	* Technical grade contains approximately 10% related; chlorinated pyridines

Use	A potent inhibitor of nitrification now in use with ammonium fertilizers; active ingredient in N-Serve nutrient stabilizer.
Molecular weight	230.9
Vapour pressure, mmHg	0.0028 at 20 °C
Water solubility, mg/l	40
Melting point, °C	62–63
Log soil sorption coefficient, log Kom	2.31 (Sabljic 1987)
Photochemical degradation in water	Photolysis products: 6-chloropicolinic acid, 6-hydroxypicolinic acid and unidentified polar material (Meikle et al. 1978).
Half-life in water, days	1.7–4.0 at 35 °C depending on concentration in distilled water 0.5 in natural water (Verschueren 1983)
Total degradation in soil	6-Chloropicolinic acid is the sole detectable metabolite, other than carbon dioxide in soil (Verschueren 1983).
Other information about degradation	50% inhibition of NH3 oxidation in Nitrosomonas at 11 mg/l (Hooper & Terry 1973).
LD50 values to mammals in oral exposure, mg/kg	1230 orl-rat 710 orl-mus 500–1000 orl-rbt (Verschueren 1983) 710 orl-mus 940 orl-rat 500 orl-rbt (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	850 skn-rbt 3113 unk-mus 3675 unk-rat (Sweet 1987)
Carcinogenicity	NCI carcinogenesis studies (IPR); clear evidence; mouse, rat (Sweet 1987).
LD50 values to birds in oral exposure, mg/kg	235 orl-ckn (Sweet 1987)

473 • 2-Chloro-6-nitrotoluene 83–42–1

Synonyms	6-Chloro-2-nitrotoluene Benzene, 1-chloro-2-methyl-3-nitro-
Sumformula of the chemical	C7H6ClNO2
EINECS–number	2014759
EC50 values to microorganism, mg/l	1.84 15 min, Photobacterium phosphoreum (Anon. 1986b)
EC50 values to algae, mg/l	6.8 96hr, grw, Chlorella pyrenoidosa (AQUIRE 1994)
NOEC values to crustaceans, mg/l	0.63 21d, rpd, Daphnia magna (AQUIRE 1994)
LC50 values to fishes, mg/l	5.2 14d, Poecilia reticulata (AQUIRE 1994)

474 • 2-Chloro-N,N-diethyl-3-hydroxycrotonamide, dimethyl phosphate 13171-21-6

Synonyms	Phosphoric acid, dimethyl ester, ester with 2-chloro-N,N-diethyl-3-hydroxycrotonamide 0,0-Dimethyl-0-(2-chloro-2-(N,N-diethylcarbamoyl)-1-methylvinyl phosphate Famfos Fosfamidon Phosphamidon 1-Chloro-diethylcarbamoyl-1-propen-2-yl dimethyl phosphate
Sumformula of the chemical	C10H19ClNO5P
Use	Insecticide, acaricide.
Molecular weight	299.72
LD50 values to mammals in oral exposure, mg/kg	15 orl-rat 17 orl-rat 6 orl-mus 9.04 orl-ckn 3.81 orl-dck 2 orl-bwd (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	125 skn-rat 26 scu-rat 6 ivn-mus 267 skn-rbt 26 skn-dck (Lewis & Sweet 1984)
LC50 values to mammals in inhalation exposure, mg/m³	135 ihl-rat (Lewis & Sweet 1984)
TDLo values to mammals in oral exposure, mg/kg	5400 orl-rat (Lewis & Sweet 1984)
Other information about mammals	ALD = 18 mg/kg, act, orl, deer mouse; LDfr = 50 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).
Carcinogenicity	NCI carcinogenesis bioassay completed: results indefinite, rat; results negative, mus (Lewis & Sweet 1984).
LD50 values to birds in oral exposure, mg/kg	2 orl-bwd 3.81 orl-dck (Lewis & Sweet 1984)
LD50 values to birds in dermal exposure, mg/kg	26 skn-dck (Lewis & Sweet 1984)
LC50 values to crustaceans, mg/l	0.0088 48hr, Daphnia pulex (Sanders & Cope 1966) 0.0028 96hr, Gammarus lacustris (Sanders 1969) 1.63 48hr, Macrobrachium lamerrei (Nagabhushanam et al. 1983) 0.0125 act, Daphnia magna (Kenaga 1979)
LC50 values to fishes, mg/l	5 24hr, Salmo gairdneri (Edwards 1977) 4.5 96hr, Lepomis macrohirus (Verschueren 1983) 10.5 96hr, Channa striata (Choudhuri et al. 1984) 8 act, Salmo gairdneri (Kenaga 1979)

C

475 • Chloro-n-paraffin (C=8-22) 61788-76-9

Sumformula of the chemical	CnH2n+2-xClx
Bioconcentration factor, fishes	90–110 8w, Cyprinus carpio, conc 0.36 mg/l 300–450 8w, Cyprinus carpio, conc 0.036 mg/l (MITI 1992)
LC50 values to fishes, mg/l	120 48hr, Oryzias latipes (MITI 1992)

476 • 4-Chloro-o-cresol 1570-64-5

Synonyms	4-Chloro-2-cresol 4-Chloro-6-methylphenol 4-Chloro-2-methylphenol
Sumformula of the chemical	C7H7ClO
Products containing the chemical	MCPA * impurity in technical grade MCPA
Molecular weight	142.59
Water solubility, mg/l	> 1000 (MITI 1992)
Melting point, °C	48 (MITI 1992)
Log octanol/water coefficient, log Pow	3.12 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	8.2–28 6w, Cyprinus carpio, conc 0.02 mg/l 6.4–14 6w, Cyprinus carpio, conc 0.002 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	1320 orl-mus (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	56 ivn-mus (Sweet 1987)
LC50 values to crustaceans, mg/l	0.29 48hr, Daphnia magna (LeBlanc 1980)
LC50 values to fishes, mg/l	2.1 24hr, Salmo trutta (Hattula et al. 1979) 2.3 96hr, Lepomis macrochirus (Buccafusco et al. 1981) 6.3 48hr, Oryzias latipes (MITI 1992)
Other information	Metabolic product of MCPA (Hattula et al. 1979). Impurity in MCPA (Verschueren 1983).

477 • 3-Chloroacetanilide 588-07-8

Sumformula of the chemical	C8H8ClNO
Log soil sorption coefficient, log Kom	1.62 (Sabljic 1987)

478 • Chloroacetic acid

79-11-8

Synonyms	Monochloroacetic acid	
Molecular weight	94.5	
Melting point, °C	62	(MITI 1992)
Boiling point, °C	189	(MITI 1992)
pKa	2.86	
Log octanol/water coefficient, log Pow	0.4	
Total degradation in water	Biodegradation: 65% by BOD period: 21d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	

479 • Chloroacetone

78-95-5

LC50 values to fishes, mg/l	0.7	14d, Poecilia reticulata (Hermens et al. 1984)

480 • α-Chloroacetophenone

532-27-4

Synonyms	Phenacylchloride	
Odour	Characteristic; apple blossom odour; hedonic tone: strong lacrimator; Threshold Odour Concentration: 0.1 mg/m³ = 0.016 ppm, 0.1–0.7 mg/m³; Odour Index: 330 at 20 °C (Verschueren 1983).	
Molecular weight	154.59	
Specific gravity (water=1)	1.324	at 15/4 °C
Vapour density (air=1)	5.32	
Conversion factor, 1 ppm in air=	6.43	mg/m³
Conversion factor, 1 mg/m³ in air=	0.16	ppm
Vapour pressure, mmHg	0.004 0.014	20 °C 30 °C
Melting point, °C	59–60	
Boiling point, °C	244–247	
Other effects on aquatic ecosystems	Reduction of amenities: faint odour: 0.0085 mg/l (Verschueren 1983).	

481 • 2-Chloroaniline

95-51-2

Synonyms	o-Chloroaniline 2-Chlorophenylamine o-Aminochlorobenzene

Use	Intermediate.
Molecular weight	127.57
Specific gravity (water=1)	1.213 at 20/4 °C
Water solubility, mg/l	0.8 (MITI 1992)
Boiling point, °C	208–210 (MITI 1992)
Log octanol/water coefficient, log Pow	1–9 (Anon. 1988)
Henry's law constant, Pa x m³/mol	0.32 (Anon. 1988)
Mobility	Equilibrium distribution: *mass %* air 9.95 water 88.97 solid 1.08 (Anon. 1988).
Total degradation in soil	Decomposition by soil microflora: > 64 days (Verschueren 1983).
Total degradation in water	Biodegradation: 2.7% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Other information about degradation	Degradation by Aerobacter: 500 mg/l at 30 °C: parent: 100% ring disruption in 60hr; mutant: 100% ring disruption in 18hr (Verschueren 1983).
Bioconcentration factor, fishes	5.4–9.0 8w, Cyprinus carpio, conc 0.1 mg/l < 14–32 8w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to birds in oral exposure, mg/kg	100–562 orl-Agelaius phoeniceus ≥ 1000 Sturnus vulgaris ≥ 1000 Coturnix coturnix (Schafer et al. 1983)
LC50 values to fishes, mg/l	6.2 14 d, Poecilia reticulata (Hermens et al. 1985) 6.3 48hr, Oryzias latipes (MITI 1992)

482 • 3-Chloroaniline 108-42-9

Synonyms	m-Chloroaniline 3-Chlorophenylamine
Use	Intermediate for azo dyes and pigments; pharmaceuticals; insecticides; agricultural chemicals.
Molecular weight	127.57
Specific gravity (water=1)	1.216 at 20/4 °C
Vapour density (air=1)	4.41

Conversion factor, 1 ppm in air=	5.3 mg/m³
Conversion factor, 1 mg/m³ in air=	0.19 ppm
Vapour pressure, mmHg	< 0.1, at 30 °C
Melting point, °C	-10.4
Boiling point, °C	229.8
Log octanol/water coefficient, log Pow	1.88
Total degradation in soil	Decomposition period by a soil microflora: > 64 days (Verschueren 1983).
Other information about degradation	Degradation by Aerobacter: 500 mg/l at 30 °C: parent: 100% ring disruption in 68hr mutant: 100% ring disruption in 16hr (Verschueren 1983).
LD50 values to birds in oral exposure, mg/kg	133 orl-Agelaius phoeniceus > 1000 orl-Sturnus vulgaris 422 orl-Coturnix coturnix 178 orl-Passer domesticus (Schafer et al. 1983)
LC50 values to fishes, mg/l	13 14d, Poecilia reticulata (Hermens et al. 1985)
Other information about water organisms	EC50 (24hr), 100 mg/l, rpd, Tetrahymena pyriformis (Yoshioka et al. 1985).

483 • 4-Chloroaniline

106-47-8

Synonyms	4-Chlorophenylamine p-Chloroaniline
Sumformula of the chemical	C6H6ClN
Use	Dye intermediate; pharmaceuticals; agricultural chemicals.
State and appearance	Rhombic prisms.
Odour	Sweet odour.
Molecular weight	127.58
Specific gravity (water=1)	1.427 at 19/4 °C
Vapour density (air=1)	4.41
Density, kg/m³	1429 19 °C
Conversion factor, 1 ppm in air=	5.3 mg/m³
Conversion factor, 1 mg/m³ in air=	0.19 ppm
Vapour pressure, mmHg	0.015 20 °C 0.05 30 °C
Water solubility, mg/l	2900
Melting point, °C	70–72
Boiling point, °C	231–232
pKa	3.97 25 °C

Log octanol/water coefficient, log Pow	1.83 (Anon. 1986) 1.8 (Anon. 1988) 2.05 (Anon. 1989)
Henry's law constant, Pa x m³/mol	0.02 (Anon. 1988) 0.06 (Anon. 1989)
Mobility	Equilibrium distribution: *mass %* air 0.67 water 93.38 solid 0.95 (Anon. 1988). Theoretical distribution: 3.5% air 79% water 18% sediment and soil (Nordic 1988).
Photochemical degradation in water	28% photomineralized (290 nm) after 17 hours (Freitag et al. 1982).
Hydrolysis in water	Does not hydrolyse (Rippen 1988).
Aerobic degradation in soil	In the presence of soil microflora degradation takes more than 64 days (Alexander & Lustigman 1966).
Aerobic degradation in water	Surface water, 48hr: not easily degradable (Janicke & Hilge 1977).
Total degradation in soil	Decomposition period by a soil microflora: > 64 days (Verschueren 1983).
Other information about degradation	Degradation by Aerobacter: 500 mg/l at 30 °C: parent: 100% ring disruption in 59hr mutant: 100% ring disruption in 12hr (Verschueren 1983). Active sludge (aerobic): 17% mineralized in 5 days (Freitag et al. 1982). OECD-screening: 10% degradation in 28 days (Rippen 1988).
Bioconcentration factor, fishes	< 10 Leuciscus, static, 3d (Freitag et al. 1982)
Bioconcentration factor, algae	260 Chlorella, static, 24hr (Freitag et al. 1982)
Other information about bioaccumulation	Accumulation factor, active sludge, 5 days, 1300 (Freitag et al. 1982).
LD50 values to mammals in oral exposure, mg/kg	310 orl-rat 100 orl-mus (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	239 skn-cat 360 skn-rbt (Lewis & Sweet 1984)
Health effects	Man: severe toxic effects: 8 ppm = 44 mg/m³, 1 min. symptoms of illness: 4 ppm = 22 mg/m³ unsatisfactory: > 2 ppm = 11 mg/m³ (Verschueren 1983).
Carcinogenicity	NCI carcinogenesis bioassay completed: results indefinite; mus, rat (Lewis & (Sweet 1984)). Suspected carcinogen (Poirier & Weisburger 1979).
Mutagenicity	Negative in Ames test and in DNA reparation test (Rippen 1988).

LD50 values to birds in oral exposure, mg/kg	100	orl-bwd (Lewis & Sweet 1984)
	1000 237	orl-Sturnus vulgaris orl-Coturnix coturnix (Schafer et al. 1983)
Effects on invertebrates	Invertebrates; 0.080 mg/l, 15 days, population effect (change in species diversity) (Lay 1987).	
EC50 values to algae, mg/l	2.4	96hr, grw, Scenedesmus subspicatus (Geyer et al. 1985)
	2.2–2.4	algae, 72hr (Rudolph & Boje 1988)
EC50 values to crustaceans, mg/l	0.042	14d, Daphnia magna, rpd (Hattori et al. 1984)
	0.06	72hr, Daphnia (Rippen 1988)
LOEC values to crustaceans, mg/l	0.0043	21d, rpd, Daphnia, Rudoph & Boje 1988
LC50 values to fishes, mg/l	12 14 2	96hr, Pimephales promelas 96hr, Salmo gairdneri 96hr, Lepomis macrochirus (Julin & Sanders 1978)
	26	14d, Poecilia reticulata (Hermens et al. 1984)
	4.6	96hr, Leuciscus (Rudolph & Boje 1988)
LOEC values to fishes, mg/l	3.2	21d, Leuciscus (Rudolph & Boje 1988)

484 • 4-Chloroanisole

623-12-1

Sumformula of the chemical	C7H7ClO	
EC50 values to microorganism, mg/l	3.2	Microtox (Kaiser et al. 1985)

485 • 1-Chloroanthraquinone

82-44-0

Sumformula of the chemical	C14H7ClO2	
EINECS-number	2014214	
Total degradation in water	Biodegradation: 2.8% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).	
Bioconcentration factor, fishes	135–351 118–282	8w, Cyprinus carpio, conc 0.24 mg/l 8w, Cyprinus carpio, conc 0.024 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	23.5	48hr, Oryzias latipes (MITI 1992)

486 • 2-Chloroanthraquinone 131-09-9

Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	81–249 93–289	8w, Cyprinus carpio, conc 0.2 mg/l 8w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LD50 values to birds in oral exposure, mg/kg	> 316 > 316	orl-Agelaius phoeniceus orl-Sturnus vulgaris (Schafer et al. 1983)
LC50 values to fishes, mg/l	30	48hr, Oryzias latipes (MITI 1992)

487 • 2-Chlorobenzaldehyde 89-98-5

Synonyms	o-Chlorobenzaldehyde	
Molecular weight	140.57	
Specific gravity (water=1)	1.248	
Melting point, °C	10–11.5	
Boiling point, °C	209–215	
Log octanol/water coefficient, log Pow	2.19	
LC50 values to fishes, mg/l	5.2 2.5	12hr, Salmo gairdneri 96hr, Salmo gairdneri (Abram & Wilson 1979)
Other information	Hydrolysis product of o-chlorobenzylidene-malononitrile (Verschueren 1983).	

488 • Chlorobenzene 108-90-7

Synonyms	Phenylchloride Monochlorobenzene Benzene chloride Chlorbenzene MCB
Sumformula of the chemical	C6H5Cl
Use	Intermediate in dyestuffs manufacturing; manufacturing aniline; insecticide; phenol; solvent.
State and appearance	Colourless liquid.

C

Odour	Characteristic; chlorinated mothballs, aromatic. Human odour perception: 0.4 mg/m³ = 0.09 ppm; human reflex response: no response: 0.1 mg/m³ adverse response: 0.2 mg/m³ animal chronic exposure: no effect: 0.1 mg/m³ adverse effect: 1.0 mg/m³ (Stern 1968). Odour index: 52600, 20 °C (Verschueren 1983).
Molecular weight	112.56
Specific gravity (water=1)	1.1066 at 20/4 °C
Vapour density (air=1)	3.88
Conversion factor, 1 ppm in air=	4.678 mg/m³
Conversion factor, 1 mg/m³ in air=	0.217 ppm
Vapour pressure, mmHg	8.8 20 °C 11.8 25 °C 15 30 °C
Water solubility, mg/l	500 20 °C 488 30 °C 502 25 °C (Banerjee 1984)
Melting point, °C	-45.6 (Suntio et al. 1988) -45 (MITI 1992)
Boiling point, °C	131–132 (MITI 1992)
Log octanol/water coefficient, log Pow	2.84 20 °C (Anon. 1986) 2.18–3.79 (Sabljic 1987) 2.84 (Chin et al. 1986) 2.98 (Anon. 1988) 2.71 (Schwarzenbach & Westall 1981) 2.84 (Hansch & Leo 1979) 2.83 (Yalkowsky 1979) 2.81 (Konemann et al. 1979) 2.98 (Miller et al. 1984) 2.63 (Mackay et al. 1979) 3.79 (Mackay 1982) 2.84 (Sangster 1989)
Log organic C/water coefficient, log Pcw	2.59 exptl. (Schwarzenbach & Westall 1981) 2.44 calc. (Schwarzenbach & Westall 1981)
Henry's law constant, Pa x m³/mol	367.7 calc. (Mackay et al. 1979) 382 exptl. (Mackay et al. 1979) 460 calc. (Yaws et al. 1991)
Mobility	Equilibrium distribution: *mass %* air 99.45 water 0.48 solid 0.07 (Anon. 1988).

C

Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 30 mg/l sludge:100 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Other information about degradation	Impact on biodegradation processes: at 100 mg/l, no inhibition of NH_3 oxidation by Nitrosomonas sp. (Hockenbury & Grady 1977). Degradation of chlorobenzene:

ENVIRONMENT	*INIT.CONC. mg/l*	*REDOX-COND.*	*TEMP. °C*	*DEGRADATION %/day*	*REF.*
water	200	aerobic	30	100/58	a
water	5	aerobic	25	49/7	b
water	10	aerobic	25	37/7	b
water (adapted)	5	aerobic	25	100/7	b
water (adapted)	10	aerobic	25	95/7	b
groundwater	0.01	aerobic	-	91/20	c
groundwater	0.01	sulfate reducing	-	0/1000	c
groundwater	0.01	nitrate reducing	-	0/1000	c
groundwater	0.01	methanogen	-	0/1000	c
sediment	< 0.0001	methanogen	20	0/230	d

a) Verschueren 1983 b) Tabak et al. 1981
c) Bouwer 1987 d) Horowitz et al. 1982

Bioconcentration factor, fishes	4.3–40 8w, Cyprinus carpio, conc 0.15 mg/l 3.9–23 8w, Cyprinus carpio, conc 0.015 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	2910 orl-rat 2830 orl-rbt (Lewis & Sweet 1984) 5060 orl-gpg 2250 orl-rbt (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	515 ipr-mus (Sweet 1987)
LC50 values to mammals in inhalation exposure, ppm	12000 ihl-rat, 30 min. 8000 ihl-cat, 30 min. (Verschueren 1983)
LDLo values to mammals in oral exposure, mg/kg	250 orl-mus (Sweet 1987)
LDLo values to mammals in non-oral exposure, mg/kg	4100 ipr-gpg 7400 ipr-rat 7000 scu-rat (Sweet 1987)
LCLo values to mammals in inhalation exposure, mg/kg	15000 ihl-mus (Lewis & Sweet 1984) 15 ihl-mus (Sweet 1987)

TCLo values to mammals in inhalation exposure, ppm	75	ihl-rat, 6hr, 6-15d preg. specific developmental abnormalities
	210	ihl-rat, 6hr, 6-15d preg. specific developmental abnormalities
	590	ihl-rbt, 6hr, 6-18d preg. effects on fertility
	10	ihl-rbt, 6hr, 6-18d preg. specific developmental abnormalities (Sweet 1987)
Other information about mammals	Rabbits: oral dose: no effect, 14.4 mg/kg, 192 days; Rabbits: oral dose: slight dip in growth, 144 mg/kg, 192 days (Verschueren 1983). Guinea pigs: inhalation: no effect, 200 ppm, 7hr/day, 5 days/week, 44 days; cat: inhalation; death after 7hr, 3700 ppm; cat; inhalation: tolerated for 1hr, 220–660 ppm (Patty 1967).	
Health effects	Man: severe toxic effects; 400 ppm = 1872 mg/m³, 60 min. symptoms of illness: 200 ppm = 936 mg/m³, 60 min. (Verschueren 1983).	
Carcinogenicity	NTP carcinogenesis studies (gavage); some evidenxe: rat; no evidenxe: mouse (Sweet 1987).	
Maximum longterm immission concentration in air for plants,mg/m³	5	VDI 2306
Maximum longterm immission concentration in air for plants,ppm	1	VDI 2306
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 17 mg/l (Bringmann & Kühn 1980a).	
EC50 values to microorganism, mg/l	15	min Microtox (Hermens et al. 1985)
	410	0.5hr, Resazurin reduction, methanol
	400	0.5hr, Resazurin reduction, ethanol
	400	0.5hr, Resazurin reduction, acetone
	470	0.5hr, Resazurin reduction, DMSO (Thompson et al. 1986)
EC50 values to algae, mg/l	12.5	96hr, growth, Selenastrum capricornutum
	33	3hr, photosynthesis, Selenastrum capricornutum (Calamari et al. 1983)
LOEC values to algae, mg/l	120	Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to crustaceans, mg/l	86	48hr, Daphnia magna (LeBlanc 1980)
	4	16d, Daphnia magna (Hermens et al. 1984)
	4.3	24hr, Daphnia magna (Calamari et al. 1983)
EC50 values to crustaceans, mg/l	4.3	srv, 24hr, Daphnia magna (Calamari et al. 1983)
	1.1	rpd, 16d, Daphnia magna (Hermens et al.)
NOEC values to crustaceans, mg/l	1	16d, srv, Daphnia magna
	0.32	16d, rpd, Daphnia magna (Hermens et al. 1984)

LC50 values to fishes, mg/l	0.05–0.35	96hr, Micropterus salmoides (Birge et al. 1979)
	29	96hr, Pimephales promelas
	24	96hr, Lepomis macrochirus
	45	96hr, Poecilia reticulata (Jones 1971)
	16	96hr, Lepomis macrochirus (Buccafusco et al. 1981)
	4.7	96hr, Salmo gairdneri (Dalich et al.1982)
	4.1	48hr, Salmo gairdneri
	10.5	48hr, Brachydanio rerio (Calamari et al. 1983)
	17	48hr, Oryzias latipes (MITI 1992)
Other information about water organisms	LD50 (24hr), 1.8 ml/kg, Salmo gairdneri (Verschueren 1983). Toxicity threshold (cell multiplication inhibition test): algae (Microcystis aeruginosa): 120 mg/l (Bringmann & Kühn 1976) green algae (Scenedesmus quadricauda): > 390 mg/l protozoa (Entosiphon sulcatum): > 390 mg/l (Bringmann & Kühn 1980a) protozoa (Uronema parduczi): > 392 mg/l (Bringmann & Kühn 1980b).	
Other effects on aquatic ecosystems	Reduction af amenities: Threshold Odour Concentration: 0.1 mg/l (Verschueren 1983).	

489 • 4-Chlorobenzenesulfonamide 98-64-6

Synonyms	1-Chloro-4-benzenesulfonamide	
EC50 values to microorganism, mg/l	69.3	Microtox (Kaiser et al. 1985)

490 • p-Chlorobenzenesulfonic acid 5138-90-9

Molecular weight	192.62	
Melting point, °C	68	
Boiling point, °C	147–148, at 25 mm	
Total degradation in soil	Decomposition period by a soil microflora (Verschueren 1983).	
LC50 values to crustaceans, mg/l	2150	96hr, Daphnia magna (Dowden & Bennet 1965)
LC50 values to fishes, mg/l	3219	24hr, Lepomis macrochirus (Freeman 1953)

491 • 4-Chlorobenzhydrol 119-56-2

Synonyms	Benzenemethanol, 4-chloro-a-phenyl-	
Sumformula of the chemical	C13H11ClO	
EINECS-number	2043334	
Water solubility, mg/l	71	(MITI 1992)
Melting point, °C	60–61.5	(MITI 1992)

Log octanol/water coefficient, log Pow	3.61	(MITI 1992)
Bioconcentration factor, fishes	34–77 34–89	8w, Cyprinus caarpio, conc 0.2 mg/l 8w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
LC50 values to fishes, mg/l	37.4	48hr, Oryzias latipes (MITI 1992)

492 • 4-Chlorobenzhydryl chloride

134-83-8

Synonyms	Benzene, 1-chloro-4-(chlorophenylmethyl)-	
Sumformula of the chemical	C13H10Cl2	
EINECS-number	2051586	
Melting point, °C	< -10	(MITI 1992)
Boiling point, °C	159–160	(MITI 1992)
Total degradation in water	Biodegradation: 0–1% by BOD (dechlorinated to 4-Chlorobenzhydrol) period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

493 • 2-Chlorobenzoic acid

118-91-2

Synonyms	o-Chlorobenzoic acid	
Molecular weight	156.57	
Specific gravity (water=1)	1.544	at 20/4 °C
Water solubility, mg/l	2100	at 25 °C
Melting point, °C	141.5	(MITI 1992)
Log octanol/water coefficient, log Pow	1.98	
Total degradation in soil	Decomposition period by a soil microflora: > 64 days (Verschueren 1983).	
Total degradation in water	Biodegradation: 5.6% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).	
Bioconcentration factor, fishes	< 1 < 10	6w, Cyprinus carpio, conc 1.25 mg/l 6w, Cyprinus carpio, conc 0.125 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	> 500	orl-rbt (Patty 1967)
LC50 values to fishes, mg/l	255	48hr, Oryzias latipes (MITI 1992)

494 • 3-Chlorobenzoic acid 535-80-8

Synonyms	m-Chlorobenzoic acid	
Molecular weight	156.57	
Specific gravity (water=1)	1.496	at 25/4 °C
Water solubility, mg/l	400	0 °C
Melting point, °C	158	
Log octanol/water coefficient, log Pow	2.68	Anon. 1986
Total degradation in soil	Decomposition period by a soil microflora: 32 days (Verschueren 1983).	
LD50 values to mammals in oral exposure, mg/kg	> 500	orl-rbt (Patty 1967)

495 • 4-Chlorobenzoic acid 74-11-3

Synonyms	p-Chlorobenzoic acid	
Molecular weight	156.57	
Specific gravity (water=1)	1.541	at 24/4 °C
Water solubility, mg/l	77	25 °C
Melting point, °C	243	
Log octanol/water coefficient, log Pow	2.65	
Total degradation in soil	Decomposition period by a soil microflora: 64 days (Verschueren 1983).	
EC50 values to microorganism, mg/l	6.2	Microtox (Kaiser et al. 1985)

496 • 4-Chlorobenzophenone 134-85-0

EC50 values to microorganism, mg/l	1.1	Microtox (Kaiser et al. 1985)

497 • p-Chlorobenzyl-pseudothiuronium chloride 544-47-8

Other information about mammals	LDfr = 62.5 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

498 • 4-Chlorobenzylamine 104-86-9

EC50 values to microorganism, mg/l	14.1	Microtox (Kaiser et al. 1985)

499 • 4-Chlorobenzylchloride 104-83-6

EC50 values to microorganism, mg/l	0.5	Microtox (Kaiser et al. 1985)

500 • 4-Chlorobenzoylchloride 122-01-0

EC50 values to microorganism, mg/l	4.8	Microtox (Kaiser et al. 1985)

501 • o-Chlorobenzylidene malononitrile 2698-41-1

Molecular weight	188.62	
Vapour density (air=1)	6.52	
Conversion factor, 1 ppm in air=	7.84	mg/m³
Conversion factor, 1 mg/m³ in air=	0.13	ppm
Melting point, °C	95	
Boiling point, °C	310–315 315	
Hydrolysis in water	o-chlorobenzylidene malononitrile + H2O ↔ o-chlorobenzaldehyde + malononitrile	
LC50 values to fishes, mg/l	1.28 0.22	12hr, Salmo gairdneri 96hr, Salmo gairdneri (Abram & Wilson 1979)

502 • 2-Chlorobiphenyl 2051-60-7

Sumformula of the chemical	C12H9Cl	
Water solubility, mg/l	5.8	
Log octanol/water coefficient, log Pow	3.90–4.59 4.5 4.52	(Sabljic 1987) (Chin et al. 1986) (Sangster 1989)
Other information about degradation	Biodegradation: 100% degradation after 1 hour by Alcaligenes Y42 (cell number 200000000/ml) and Acinetobacter P6 (cell number 44000000/ml) at 9.3 mg/l initial concentration, trimethylsilyl derivative of monochlorobenzoic acid was detected in the metabolite (Verschueren 1983).	
Other information about bioaccumulation	Marine yeast Rhodotorula rubra: bioconcentration coefficient: 737 in whole cells; 37000 in their lipid portion (Cole et al. 1979).	

503 • 3-Chlorobiphenyl 2051-61-8

Sumformula of the chemical	C12H9Cl	
Water solubility, mg/l	3.3	
Log octanol/water coefficient, log Pow	4.58	(Sangster 1989)
Other information about degradation	Biodegradation: 100% degradation after 1 hour by Alcaligenes Y42 (cell number 200000000/ml) and Acinetobacter P6 (cell number 44000000/ml) at 9.3 mg/l initial concentration, trimethylsilyl derivative of monochlorobenzoic acid was detected in the metabolite (Verschueren 1983).	
Other information about bioaccumulation	Marine yeast Rhodotorula rubra: bioconcentration coefficient: 1180 in whole cells; 59000 in their lipid portion (Cole et al. 1979).	

C

504 • 4-Chlorobiphenyl 2051-62-9

Sumformula of the chemical	C12H9Cl
Molecular weight	188.66
Water solubility, mg/l	0.8
Melting point, °C	76–78
Boiling point, °C	282
Log octanol/water coefficient, log Pow	4.26 (Mackay 1982) 4.61 (Sangster 1989)
Other information about degradation	Biodegradation: Eighteen lichens from a variety of habitats were treated with 4-CB, all were shown to partially convert 4-CB to 4-chloro-4'-hydroxybiphenyl – it took between 6 and 22 hours for the hydroxy derivative to appear. Only one species (Pseudocyphellaria crocata) produced a further metabolite: 4-chloro-4'-methoxybiphenyl (Maass et al. 1976). Biodegradation: 100% degradation after 1 hour by Alcaligenes Y42 (cell number 200000000/ml) and Acinetobacter P6 (cell number 44000000/ml) at 9.3 mg/l initial concentration, trimethylsilyl derivative of monochlorobenzoic acid was detected in the metabolite (Verschueren 1983).
Other information about bioaccumulation	Marine yeast Rhodotorula rubra: bioconcentration coefficient: 1550 in whole cells; 77500 in their lipid portion (Cole et al. 1979).

505 • Chlorocyclohexane 542-18-7

Water solubility, mg/l	500	(MITI 1992)
Melting point, °C	-43.9	(MITI 1992)
Boiling point, °C	143	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).	
Bioconcentration factor, fishes	75–240 140–297	8w, Cyprinus carpio, conc 0.0002 mg/l 8w, Cyprinus carpio, conc 0.00002 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	23.5	48hr, Oryzias latipes (MITI 1992)

506 • Chlorodifluoromethane 75-45-6

Sumformula of the chemical	CHClF2	
EINECS-number	2008719	
Water solubility, mg/l	3350	(MITI 1992)
Melting point, °C	-160	(MITI 1992)
Boiling point, °C	-40.8	(MITI 1992)

Log octanol/water coefficient, log Pow	1.13	(MITI 1992)
Total degradation in water	Biodegradation (Close Bottle test): 0% by BOD period: 28d substance: 1.69 mg/l sludge: 2mg(As)/l 2% by BOD period: 28d substance: 4.18 mg/l sludge: 2 mg(As)/l (MITI 1992).	

507 • Chlorodiphenyl methane

90-99-3

Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

508 • Chloroethane

75-00-3

Sumformula of the chemical	C2H5Cl	
Use	Solvent.	
Water solubility, mg/l	4470 7400	20 °C (MITI 1992)
Melting point, °C	-142.5	(MITI 1992)
Boiling point, °C	12.5	(MITI 1992)
Log octanol/water coefficient, log Pow	1.43 1.39	(Sangster 1989) (MITI 1992)
Henry's law constant, Pa x m³/mol	701.1	calc. (Yaws et al. 1991)
Total degradation in water	Biodegradation: 1% by BOD period: 28d substance: 1.84 mg/l sludge 2 mg/l 1% by BOD period: 28d substance: 4.19 mg/l sludge: 2 mg/l (MITI 1992).	
LC50 values to fishes, mg/l	40 19 36	96hr, Pimephales promelas 96hr, Carassius auratus 96hr, Salmo gairdneri (Phipps & Holcombe 1985)

509 • 2-Chloroethanol

107-07-3

Synonyms	β-Chloroethylalcohol Ethylenechlorohydrin Glycolchlorohydrin
Sumformula of the chemical	C2H5OCl

State and appearance	Colourless liquid.	
Molecular weight	80.52	
Specific gravity (water=1)	1.121	at 20/4 °C
Vapour density (air=1)	2.78	
Conversion factor, 1 ppm in air=	3.29	mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.304	ppm
Vapour pressure, mmHg	4.9 10	20 °C 30 °C
Melting point, °C	67.5–71	
Boiling point, °C	128.8	
LD50 values to mammals in oral exposure, mg/kg	72–95 110	orl-rat orl-gpg (Patty 1967)
Other information about mammals	Rat: inhalation: survived; 3.0 mg/l, 0.25hr; Mouse: inhalation: survived: 1.0 mg/l, 2hr (Patty 1967).	
Health effects	Man: readily penetrates the skin; severe toxic effects: 20 ppm = 68 mg/m^3, 60 min; symptoms of illness: 10 ppm = 34 mg/m^3, unsatisfactory: 2 ppm = 7 mg/m^3 (Verschueren 1983).	
EC50 values to microorganism, mg/l	391	Microtox (Nacci et al. 1986)
LC50 values to crustaceans, mg/l	> 80.9	96hr, Orconectes nais (Phipps & Holcombe 1985)
LC50 values to fishes, mg/l	39.5 35.6 19.1 26.4 21.5	96hr, Pimephales promelas 96hr, Salmo gairdneri 96hr, Carassius auratus 96hr, Ictalurus punctatus 96hr, Lepomis macrochirus (Phipps & Holcombe 1985)
Other information about water organisms	LC50, > 80.9 mg/l, 96hr, snail (Phipps & Holcombe 1985)	

510 • 2-Chloroethyl vinyl ether 110-75-8

LC50 values to fishes, mg/l	350	96hr, Lepomis macrochirus (Buccafusco et al. 1981)

511 • 2-Chloroethylbenzhydryl ether 32669-06-0

Sumformula of the chemical	C15H15OCl	
Water solubility, mg/l	< 10	(MITI 1992)
Melting point, °C	27–28	(MITI 1992)
Boiling point, °C	139–142	3-5 mmHg (MITI 1992)
Log octanol/water coefficient, log Pow	4.38	(MITI 1992)

Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	196–713 8w, Cyprinus carpio, conc 0.02 mg/l 104–549 8w, Cyprinus carpio, conc 0.002 mg/l (MITI 1992)
LC50 values to fishes, mg/l	2.15 48hr, Oryzias latipes (MITI 1992)

512 • Chloroform

67-66-3

Synonyms	Trichloromethane	
Sumformula of the chemical	CHCl3	
Use	Manufacturing fluorocarbon refrigerants and propellants and plastics; manufacturing anesthetics and pharmaceuticals, primary source for chlorodifluoromethane; fumigant; sweetener; fire extinguisher manufacturing; electronic circuitry manufacturing; analytical chemistry; insecticide; solvent.	
State and appearance	Colourless liquid.	
Odour	Odour index at 20 °C: 70 (Verschueren 1983).	
Molecular weight	119.37	
Specific gravity (water=1)	1.489	20 °C
Vapour density (air=1)	4.12	
Conversion factor, 1 ppm in air=	4.96	mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.2	ppm
Vapour pressure, mmHg	160 245	20 °C 30 °C
Water solubility, mg/l	9300 10000 8100 5000	25 °C 15 °C 20 °C (Anon. 1986b) (MITI 1992)
Melting point, °C	-63.5	(MITI 1992)
Boiling point, °C	61–62 °C 61.2	(Anon. 1986b) (MITI 1992)
Log octanol/water coefficient, log Pow	1.97 1.97 1.97 1.97 1.94 1.9 1.95	20 °C (Anon. 1986b) (Schwarzenbach et al. 1983) (Hansch & Leo 1979) (Hansch & Leo 1979) (Banerjee et al. 1980) (Mackay 1982)
Henry's law constant, Pa x m^3/mol	322 372 410.7	exptl. (Dilling 1977) exptl. (Gossett 1987) calc. (Yaws et al. 1991)

Volatilization	Measured half-life for evaporation from 1 ppm aqueous solution, still air, and an average depth of 6.5 cm: at 1–2 °C: 34.5 min.; at 25 °C: 18.5–25.7 min. (Dilling 1977).
Mobility	97.64% (air), 2.28% (water), 0.07% (sediment).
Half-life in water, days	0.012 = 18.5–25.7 min. 0.018 measured, 1 ppm aqueous liquid, 25 °C
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance 100 mg/l sludge 30 mg/l (MITI 1992).
Other information about degradation	see below

ENVIRONMENT	*INIT.CONC. mg/l*	*REDOX-COND.*	*TEMP. °C*	*DEGRADATION %/day*	*t1/2*	*REF.*
biofilm	0.028	methanogen	22	-	8 (1)	a
water	0.003	methanogen	35	93/112	11	b
water	0.029	methanogen	35	99/112	16	b
water	0.117	methanogen	35	71/112	63	b
water	0.013	aerobic	20	0/175	> 175	b
water	0.029	aerobic	20	0/175	> 175	b
water	0.080	aerobic	20	0/175	> 175	b
biofilm	0.03	aerobic	22	0/730	-	c
biofilm	0.04	methanogen	22	95/60	15	d
water	0.06	denitrif.	25	0/56	> 56	e
biofilm	0.16	methanogen	23	-	33 (1)	f
water (deion.)	1.0	aerobic	25	-	450	g
soil	0.21	aerobic + natural gas		-	0.05	h
digestive sludge	238.4	methanogen		5/90	1216	i
dig. sludge	119.2	sulfate reducing		30/90	175	i
water (adapted)	0.354	aerobic		97/11	< 2–3	i
water (abiotic)	-	aerobic	25	-	3500 yr	j
water	5–10	aerobic	25	47/7	-	k
water (adapted)	5–10	-	25	100/7	< 1	k
soil column	0.90	aerobic	20	5/2	27	l
soil column	0.25	aerobic	20	8/2	17	l
soil	0.6–0.8	aerobic	17	< 3/7	> 160	m

(1) biomass concentration set to 0.100 mg/l.

a) Bouwer & McCarty 1985
b) Bouwer et al. 1981
c) Bouwer & McCarty 1982
d) Bouwer & McCarty 1983a
e) Bouwer & McCarty 1983b
f) Bouwer & Wright 1987
g) Dilling et al. 1975
h) Anon. 1987b
i) Kästner 1986 (1000000000 org./ml)
j) Schwarzenbach 1985
k) Tabak et al. 1981
l) Wilson et al. 1981
m) Wilson et al. 1983b
(Anon. 1987b).

Bioconcentration factor, fishes	1.4–4.7 14d, Lepomis macrochirus (Anon. 1986b) 6w, Cyprinus carpio, conc 1 mg/l 4.1–13 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)

Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
	LD50 values to mammals in oral exposure, mg/kg:	
	908	orl-rat (Lewis & Sweet 1984)
	36	orl-mus (Lewis & Sweet 1984)
	800	orl-rat (Anon. 1986b)
LDLo values to mammals in oral exposure, mg/kg	140	orl-hmn (Lewis & Sweet 1984)
	2400	orl-mus (Anon. 1986b)
	1000	orl-dog (Anon. 1986b)
TCLo values to mammals in inhalation exposure, mg/kg	1000	1y, ihl-hmn (Lewis & Sweet 1984)
Health effects	Man: severe toxic effects: 2000 ppm = 9960 mg/m³, 60 min; symptoms of illness: 500 ppm = 2490 mg/m³; unsatisfactory: > 50 ppm = 249 mg/m³ (Verschueren 1983).	
Carcinogenicity	NCI carcinogenesis bioassay completed: results positive; mus, rat (Lewis & Sweet 1984).	
Maximum longterm immission concentration in air for plants,mg/m³	10	VDI 2306
Maximum longterm immission concentration in air for plants,ppm	2	VDI 2306
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 125 mg/l (Bringmann & Kühn 1980a).	
	EC50 = 435 mg/l, 5 min, Photobakterium phosphoreum, EC50 = 1013 mg/l, 5 min, Photobakterium phosphoreum (Anon. 1986b)	
EC50 values to algae, mg/l	500	24hr, assimilationtest (Anon. 1986b)
LOEC values to algae, mg/l	185	srv, Microcystis aeruginosa (Bringmann & Kühn 1976)
	1100	act, Scenedesmus quadricauda (Bringman & Kühn 1980a)
LC50 values to crustaceans, mg/l	29	48hr, Daphnia magna (LeBlanc 1980)
	28.9	48hr, Daphnia magna (Anon. 1986b)
EC50 values to crustaceans, mg/l	2140	24hr, Daphnia magna (Anon. 1986b)
LC50 values to fishes, mg/l	2.03	23d, Salmo gairdneri, embryos
	2.03	96hr, Salmo gairdneri (Birge et al. 1979)
	2.09	96hr, Salmo gairdneri (Black et al. 1982)
	162	48hr, 162/191 mg/l
	191	Leuciscus idus melanotus
	66.8	96hr, Salmo gairdneri
	43.8	96hr, Salmo gairdneri
	18	96hr, Salmo gairdneri
	18	96hr, Lepomis macrochirus
	115	96hr, Lepomis macrochirus
	100	96hr, Lepomis macrochirus
	51	96hr, Micropterus salmoides (Anon. 1986b)
	117	48hr, Oryzias latipes (MITI 1992)
Effects on the physiology of water organisms	Salmo gairdneri, 0.020 mg/l, 4d, change in enzyme activity (Castren & Oikari 1987).	

Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): algae (Microcystis aeruginosa): 185 mg/l (Bringmann & Kühn 1976) green algae (Scenedesmus quadricauda): 1100 mg/l protozoa (Entosiphon sulcatum): > 6560 mg/l (Bringmann & Kühn 1980a) protozoa (Uronema parduczi): > 6560 mg/l (Bringmann & Kühn 1980b). LC50 = 40 mg/l, 3d (Buto fowleri); LC50 = 35,14 mg/l, 4d, (Embryos); LC50 = 0.76 mg/l, 3d (Hyla crucifer); LC50 = 0.27 mg/l 4d (Hyla crucifer); LC50 = 28,17 mg/l, 4d, (Rana palustris); LC50 = 20,55 mg/l, 4d (Rana palustris); LC50 = 4.56 mg/l, 5d (Rana pipiens); LC50 = 4.16 mg/l, 4d (Rana pipiens) (Anon. 1986b)
Other effects on aquatic ecosystems	Reduction of amenities: Odour Thresholds: 20 mg/l; 0.1 mg/kg (Verschueren 1983).

513 • α-Chlorofumaric acid diethyl ester 10302-94-0

Sumformula of the chemical	C8H11O4Cl
Water solubility, mg/l	1500 (MITI 1992)
Boiling point, °C	87 (MITI 1992)
Total degradation in water	Biodegradation: 34.7% by BOD (on the upward trend) period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

514 • 1-Chloroheptane 629-06-1

Synonyms	Heptylchloride
Sumformula of the chemical	C7H15Cl
Odour	Threshold Odour Concentration: 0.330 mg/m³ = 59 ppb (Stochkham et al. 1969) 0.06 ppm; recognition: 157 mg/m³ (Verschueren 1983).
Molecular weight	134.65
Specific gravity (water=1)	0.8725 at 20/0 °C
Melting point, °C	-69.5
Boiling point, °C	159.5
Log octanol/water coefficient, log Pow	4.15 (Sangster 1989)

515 • Chlorohexidine 55-56-1

LC50 values to crustaceans, mg/l	0.25	48hr, Daphnia magna (Sanders & Cope 1966, Frear & Boyd 1967)
LC50 values to fishes, mg/l	0.0013	96hr, Salmo gairdneri (Macek & McAllister 1970)

516 • Chloromethyl methyl ether 107-30-2

Synonyms	Chloromethoxymethane Monochlorodimethylether Chloromethylether CMME
Sumformula of the chemical	C2H5OCl
Known impurities	dichloromethylether * 1-8%
Use	Manufacturing irritant gases (lacrymators); chloromethylating agent; intermediate.
State and appearance	Colourless liquid.
Molecular weight	80.52
Specific gravity (water=1)	1.0625 10/4 °C
Conversion factor, 1 ppm in air=	3.29 mg/m³
Conversion factor, 1 mg/m³ in air=	0.304 ppm
Water solubility, mg/l	> 1% (MITI 1992)
Melting point, °C	-103.5 (MITI 1992)
Boiling point, °C	59.5 (MITI 1992)
Hydrolysis in water	Hydrolyses very fast with half-life < 1 sec.; extrapolated to pure water (Verschueren 1983). Reaction: ClCH2-O-CH3 + H2O --> CH3OH + HCl + CH2O (Fishbein 1979).
Total degradation in water	Biodegradation: 33% by BOD period 28d substance: 100 mg/l sludge: 30 mg/l 67% by BOD period: 28d substance: 100 mg/l sludge 30 mg/l 76% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l 80% by BOD period 28d substance: 100 mg/l sludge: 30 mg/l 83% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	500 orl-rat (Verschueren 1983)

Other information about mammals	Rat: inhalation: dangerous: 2000 ppm, 30 min 100 ppm, > 4hr oral dose : survival : 0.3 g/kg death: 1.0 g/kg
Carcinogenicity	Man: carcinogenic because the technical grade contains dichloromethylethers which are carcinogenic (Verschueren 1983)

517 • Chloromycetin 56-75-7

Synonyms	Chloramphenicol
Sumformula of the chemical	C11H12O5N2Cl2
Use	An antibiotic derived from Streptomyces venezuelae or by organic synthesis; antifungal agent.
Molecular weight	323.13
Melting point, °C	148–150

518 • 1-Chloronaphthalene 90-13-1

Sumformula of the chemical	C10H7Cl
Molecular weight	162.62
Specific gravity (water=1)	1.194 20/4 °C
Boiling point, °C	250–280
Log octanol/water coefficient, log Pow	3.9 (Sangster 1989)
Other information about degradation	Biodegradation: metabolic pathway: 1-chloronaphthalene →8-chloro-1,2-dihydroxynaphthalene → 3-chlorosalicylic acid (Verchueren 1983)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	1540 orl-rat 1091 orl-mus (Lewis & Sweet 1984)
Other information about mammals	Rat: inhalation: no effect: 37 ppm, 15 times 6hr (Cage 1970)
LC50 values to crustaceans, mg/l	1.6 48hr, Daphnia magna (LeBlanc 1980)
LC50 values to fishes, mg/l	2.3 96hr, Lepomis macrochirus (Buccafusco et al. 1981) 2.4 96hr, Cyprinodon variegatus (Heitmuller et al. 1981)
LOEC values to fishes, mg/l	0.97 srv, schr, Cyprinodon variegatus (Ward & Parrish 1980)

519 • 2-Chloronitrobenzene 88-73-3

Synonyms	o-Chloronitrobenzene 2-Nitrochlorobenzene Chloro-o-nitrobenzene 1-Chloro-2-nitrobenzene 2-Chloro-1-nitrobenzene
Sumformula of the chemical	C6H4O2NCl

State and appearance	Needles.
Odour	Odour threshold: detection: 0.015–0.020 mg/kg (Verschueren 1983)
Molecular weight	157.56
Specific gravity (water=1)	1.368 22/4 °C
Water solubility, mg/l	10 20 °C (Anon. 1986b)
Melting point, °C	32.5
Boiling point, °C	244 (Anon. 1986b) 245–246 (MITI 1992)
Log octanol/water coefficient, log Pow	2.24 (Anon. 1986b)
Total degradation in water	Biodegradation: 8.2% by BOD period: 14d substance: 30 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987)
Other information about degradation	Biodegradation: decomposition period by a soil microflora: > 64 days (Verschueren 1983)
Bioconcentration factor, fishes	7.0–20.8 8w, Cyprinus carpio, conc 0.25 mg/l 7.4–22.3 8w, Cyprinus carpio, conc 0.025 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be nonaccumulative or low accumulative (Anon. 1987)
LD50 values to mammals in oral exposure, mg/kg	135 orl-mus 288 orl-rat 280 orl-rbt (Sweet 1987) 268 orl-rat (Anon. 1986b) 135 orl-mus (Anon. 1986b) 290 orl-rat (Anon. 1986b) 457 orl-rat, female (Anon. 1986b) 270 orl-rat, male (Anon. 1986b)
TDLo values to mammals in oral exposure, mg/kg	140 orl-mus, tumorigenic 22 orl-rat, tumorigenic (Sweet 1987)
EC50 values to microorganism, mg/l	4 Microtox (Kaiser and Ribo 1985)
EC50 values to crustaceans, mg/l	15 Daphnia magna (Anon. 1986b) 3.2 7d, Daphnia magna (Anon. 1986b)
NOEC values to crustaceans, mg/l	0.1 7d, rpd, Daphnia (Anon. 1986b)
LC50 values to fishes, mg/l	1.2 96hr, Lepomis macrochirus 0.55 96hr, Menidia audens (Dawson et al. 1977a) 5–10 Leuciscus idus melanotus (Anon. 1986b) 30 4d, Poecilia reticulate (Anon. 1986b) 28 48hr, Oryzias latipes (MITI 1992)
EC50 values to fishes, mg/l	1.8 4d, Poecilia reticulate (Anon. 1986b)

520 • 4-Chloronitrobenzene

100-00-5

Synonyms	p-Chloronitrobenzene
Sumformula of the chemical	C6H4ClNO2
Molecular weight	157.56
Specific gravity (water=1)	1.52 18/4 °C
Conversion factor, 1 ppm in air=	6.55 mg/m³
Conversion factor, 1 mg/m³ in air=	0.15 mg/m³
Water solubility, mg/l	10 20 °C (Anon. 1986b)
Melting point, °C	83.5 (MITI 1992)
Boiling point, °C	239.1 (Anon. 1986b) 242.4 (MITI 1992)
Log octanol/water coefficient, log Pow	2.44 (Anon. 1986b)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Other information about degradation	Biodegradation period by a soil microflora: > 64 days Inhibition of biodegradation: at 100 mg/l, no inhibition of NH3 oxidation by Nitrosomonas sp. (Hockenbury & Grady 1977).
Bioconcentration factor, fishes	5.8–20.9 8w, Cyprinus carpio, conc 0.15 mg/l 7.5–18.1 8w, Cyprinus carpio, conc 0.0915 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	420 orl-rat (Lewis & Tatken 1980) 650 orl-mus (Lewis & Tatken 1980) 812 orl-rat (Anon. 1986b) 420 orl-rat (Anon. 1986b) 1414 orl-mus (Anon. 1986b) 280 orl-rat, 14d (Anon. 1986b)
EC50 values to microorganism, mg/l	20.7 Microtox (Kaiser and Ribo 1985)
LC50 values to crustaceans, mg/l	10 96hr, Daphnia magna (Anon. 1986b)
EC50 values to crustaceans, mg/l	13 24hr, Daphnia magna (Anon. 1986b) 14.5 24hr, Daphnia magna (Anon. 1986b)
NOEC values to crustaceans, mg/l	0.32 21d, Daphnia magna (Anon. 1986b 0.64 21d, Daphnia magna (Anon. 1986b)
LC50 values to fishes, mg/l	20 48hr, Leuciscus idus melanotus 8.3 96hr, Lepomis macrochirus 6 96hr, Salmo gairdneri (Anon. 1986b) 14.5 48hr, Oryzias latipes (MITI 1992)

521 • Chloronitrophene 1836-77-7

Synonyms	Chlornitrofen Chlornitrophen p-Nitrophenyl-2,4,6-trichlorophenyl ether 1,3,5-Trichloro-2-(4-nitrophenoxy)benzene 2,4,6-Trichlorophenyl 4-nitrophenyl ether
Sumformula of the chemical	C12H6Cl3NO3
Molecular weight	318.54
Water solubility, mg/l	0.25 (MITI 1992)
Melting point, °C	107–108 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	1000–4600 8w, Cyprinus carpio, conc 0.02 mg/l 800–1800 8w, Cyprinus carpio, conc 0.002 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be accumulated on a medium level (Anon. 1987) (2,4,6-trichlorophenyl p-nitrophenyl ether).
LD50 values to mammals in oral exposure, mg/kg	11800 orl-mus 10800 orl-rat (Sweet 1987)
LC50 values to fishes, mg/l	0.18 24hr, Cyprinus carpio (Hashimoto et al. 1982) 40 48hr, Cyprinus carpio (Toyama & Takazava 1971) 0.77 96hr, Rasbora heteromorpha (Tooby et al. 1975) 110 48hr, Oryzias latipes (MITI 1992)

522 • 1-Chlorooctane 111-85-3

Sumformula of the chemical	C8H17Cl
EINECS-number	2039155
Water solubility, mg/l	< 10 (MITI 1992)
Melting point, °C	< -30 (MITI 1992)
Boiling point, °C	181.5 (MITI 1992)
Total degradation in water	Biodegradation: 74–81% by BOD period: 28d substance: 100 mg/l, sludge: 30 mg/l (MITI 1992).

523 • Chlorophacinone 3691-35-8

Other information about mammals	ALD = 1.0–3.75 mg/kg, act, orl, Deer mouse (Virtanen & Nuuja 1987).
LD50 values to birds in oral exposure, mg/kg	> 100 orl-Agelaius phoeniceus (Schafer et al. 1983)

524 • 2-Chlorophenol 95-57-8

Synonyms	o-Chlorophenol 1-Chloro-2-hydroxybenzene	
Sumformula of the chemical	C6H5ClO	
Use	Organic synthesis. Intermediate in the manufacture of higher chlorophenols and phenolic resins. Also used in a process for extracting sulfur and nitrogen compounds from coal.	
State and appearance	Colourless liquid.	
Odour	Characteristic, medicinal. Unpleasant, penetrating. Odour threshold, water: 0.005 ppm at 20 °C and 0.001 ppm at 60 °C. 0.00033 mg/l at 30 °C and 0.0025 mg/l at 60 °C. 0.002 mg/l was the geometric mean of odour threshold responses of panel members at 25 °C (Sax 1986). The threshold for taste in water at 40 °C was 0.05 ppm (Sax 1986).	
Molecular weight	128.56	
Specific gravity (water=1)	1.241 1.265	at 18/15° C at 15.5/4 °C
Vapour pressure, mmHg	40 100	82 °C 106 °C
Water solubility, mg/l	11350 20000 800	25 °C (Banerjee et al. 1980) 25 °C (Vesala 1974) (MITI 1992)
Melting point, °C	9 9.3	(Doedens 1967) (MITI 1992)
Boiling point, °C	175	(MITI 1992)
Flashing point, °C	107.3	
pKa	8.85 8.48 8.52 (Ugland et al. 1981)	
Log octanol/water coefficient, log Pow	2.17 2.17 2.15 2.19 2.27 2.16	observed (Chin et al. 1986) (Hansch & Leo 1979) (Fuita et al. 1964) (Neely et al. 1974) (Konemann & Musch 1981) (Banerjee et al. 1980)
Henry's law constant, Pa x m³/mol	1.425	calc. (Suntio et al. 1988)

Adsorption/desorption	Sorption fo 2-chlorophenol by Bentone 24 and Bentone 18C, both organo-clays, was studied. Sorption was accomplished from solution at 20 °C, during 45 to 48 hours constant shaking periods in darkened rooms. The 2-chlorophenol concentration was 0.5 mM with 5 g Bentone in a 0.005 M KHC03 buffer. pH's examined were 7.8 (pKa 8.48, 2.3% protolysis) and 7.6 (13% protolysis). Analysis was via UV-techniques. At pH 7.8, on Bentone 24, 76.6% of the initial amount was sorbed and at pH 7.6, on Bentone 18C, 15% of the initial amount was sorbed (Sax 1986).
Mobility	18.46% (air), 77.44% (water), 4.11% (sediment). Soluble in alcohol, ether, and aqueous sodium hydroxide. Very soluble in water.
Aerobic degradation in soil	Microbial decomposition in soils was studied using the shake culture method. The medium was sterilized and had a pH of 7.2. 2-chlorophenol was added to a final concentration of 0.050 mg/ml and 4 g of freshly sampled soil was added to 100 ml of medium as an inoculum. Temperature was 30 °C and cultures were aerated on the shaker. Two soil types were used: Mardin silt loam and Dunkirk silt loam. UV spectrophotometry was used to measure persistence. Time required for the complete disapperance in Dunkirk and Mardin soils was 14 and 47 days, respectively. Information that it was microbial decomposition was tested (positive) by use of sodium azide treated samples. – Manometric analysis of different genera of soil bacteria for co-oxidation fo phenol and 2-chlorophenol indicated that three Norcardia strains, three Pseudomonad strains, a Bacillus strain, and Mycobacterium coeliacum were capable of co-oxidation. Oxidation was to either 3- or 4-chlorocatechol (Sax 1986). AEROBIC DEGRADATION IN SOIL Maximum adsorption wavelength: 275 nm NON-STERILE SOIL Minimum time for > 70% decrease: 0.50–1.00 d % decomposition at the termination of the experiment: 1.5d, 100% STERILE SOIL % decomposition at the termination of the experiment: 40d, 67% (Baker et al. 1980)
Anaerobic degradation in soil	ANAEROBIC DEGRADATION IN SOIL Maximum adsorption wavelength: 275 nm NON-STERILE SOIL Minimum time for > 70% decrease: 10–24 d % decomposition at the termination of the experiment: 80d, 78% STERILE SOIL Minimum time for > 70% decrease: 24–80 d % decomposition at the termination of the experiment: 80d, 82% (Baker et al. 1980)
Aerobic degradation in water	Degradation by Pseudomonas: 200 mg/l at 30 °C: parent: 100% ring disruption in 52hr mutant: 100% ring disruption in 26hr (Verschueren 1983)
Total degradation in soil	Decomposition rate in soil suspensions: 14 days for complete disappearance (Verschueren 1983). Decomposition period by a soil microflora: > 64 days (Verschueren 1983) Decomposition of 2-chlorophenol in soils was studied by making a solution of 1 g 2-chlorophenol in 4 l of tap water and buffers and then allowing it to percolate through Rothamsted soil. 66% disappeared in 10 days. Further additions of compound to the system showed rates of disappearance nearly twice that of the initial rate. When tested against sterilized soil the disappearance was found to have twice the rate in unsterilized soil over a period of 7 days. 0.1% sodium azide added to solutions showed no significant effects. Pretreatment with phenol showed no significant change. – Found as an intermediate in degradation of 2,4-D by two Pseudomonas strains. The proposed pathway of degradation was from 2-chlorophenol to 3-chlorocatechol to α-chloromuconic acid (Sax 1986).

Total degradation in water	In activated sludge with an initial concentration of 100 mg/l, 100% ring degradation was noted in 3 days and 100% chloride ion development was noted in 4 days. – The persistence of 2-chlorophenol in polluted river water and dilute sewage was examined at 20 °C. At an initial concentration of 1 mg/l added to a usual dilution of domestic sewage, removal was not noted over the 20–30 days period of observation, presumed to be due to lack of microorganisms capable of attacking the chemical. At the same concentration in polluted river water, dissipation was in 15–23 days. Addition of seed considerably enhanced dissipation. Results of this indicate removal by specialized microflora (Sax 1986). Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992)
Metabolism in mammals	Dogs excreted 87% of administered 2-chlorophenol as co njugated of sulfate and glucuronic acid. Rabbits also apparently conjugate 2-chlorophenol, derived from chlorobenzene exposure, in the same fashion (Sax 1986).
Metabolism in plants	The metabolic fate of 2-chlorophenol in tomato plants included glycoside formation. β-o-chlorophenylgentiobioside was isolated from the roots. No evidence for the formation of this glycoside in shoots was found (Sax 1986).
Other information about metabolism	Inhibition on degradation of glucose by Pseudomonas fluorescens at: 30 mg/l, and E. coli at: 400 mg/l (Verschueren 1983)
Bioconcentration factor, fishes	214 28d, Lepomis macrochirus whole body (Sax 1986) 14–24 6w, Cyprinus carpio, conc 0.04 mg/l 16–29 6w, Cyprinus carpio, conc 0.004 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	670 orl-rat 670 orl-mus 440 orl-mam (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	230 ipr-rat 950 scu-rat (Sax 1986)
LDLo values to mammals in non-oral exposure, mg/kg	950 scu-rbt, 120 ivn-rbt 800 scu-gpg (Sax 1986)
TDLo values to mammals in non-oral exposure, mg/kg	4800 12W-I, skn-mus, tumorigenic (Sax 1986)
Effects on the physiology of mammals	The inhibition of oxidative phosphorylation by 50% was shown at a concentration of 0.000520 M in rat liver mitochondria. Measurement was via oxygen consumption using polarographic techniques. – 2-MCP produced reversible inhibition of etiolated pea brei (a finely divided tissue suspension) catalase, and of crystalline beef liver catalase in vitro at a level of 0.00004 M (Sax 1986).
Health effects	Toxic by skin absorption, inhalation or ingestion. Strong tissue irritant. When heated to decomposition, highly toxic fumes may be emitted.
LD50 values to birds in oral exposure, mg/kg	> 113 orl-Agelaius phoeniceus (Schafer et al. 1983)
Effects on amphibia	LDLo, scu, frog, 400 mg/kg (Sax 1986).

Effects on wastewater treatment	The effect of 2-chlorophenol on respiration of activated sludge was studied using Wanburg techniques and GLC analysis. The inoculum was a mixture from 2 treatment plants that had been exposed to continuous incoming phenol in the range of 0.01–0.35 mg/l for 12 months. At concentrations of 1 mg/l, 100% degradation was noted after 3 hours, 97% degradation was seen after 6 hours at initial concentration of 10 mg/l, and only 20 % degradation after 6 hours with an initial concentration of 100 mg/l. 98% recovery was noted with the analysis, indicating little adsorption onto particulate matter (Sax 1986).	
EC50 values to microorganism, mg/l	380	OECD 209 (Klecka et al. 1985)
EC50 values to algae, mg/l	170 70	4d, grw, Chlorella vulgaris 4d, grw, Selenastrum capricornutum (Shigeoka et al. 1988)
LC50 values to crustaceans, mg/l	2.6	48hr, Daphnia magna (LeBlanc 1980)
	3.73	7d, Daphnia magna (LeBlanc et al. 1988)
EC50 values to crustaceans, mg/l	7.43 > 22 2.6	48hr, Daphnia magna 24hr, Daphnia magna 48hr, Daphnia magna (Sax 1986)
	1.35	7d, enzyme effect, Daphnia magna (LeBlanc et al. 1988)
LC50 values to fishes, mg/l	2.9	96hr, Salmo gairdneri (Voss et al. 1980)
	6.6	96hr, Lepomis macrochirus (Buccafusco et al. 1981)
	9.7 6.3	48hr, Pimephales promelas schr, Pimephales promelas (Phipps et al. 1981)
	16	24hr, Carassius auratus (Kobayashi et al. 1973)
	8.4	96hr, Lepomis macrochirus (McKee et al. 1963)
	11 8 12	96hr, Pimephales promelas 96hr, Lepomis macrochirus 96hr, Carassius auratus (Lammering & Burbank 1960)
	12.37 11.63 14.48 12.4 20.17 6.59 10 8.4	96hr, Carassius auratus 96hr, Pimephales promelas 96hr, Pimephales promelas 96hr, Pimephales promelas 96hr, Lebistes reticulata 96hr, Lepomis macrochirus 96hr, Lepomis macrochirus 96hr, Lepomis macrochirus, juv. (Sax 1986)
	9.41	4d, Pimephales promelas (Geiger et al. 1988)
	16.7	48hr, Oryzias latipes (MITI 1992)
Effects on the physiology of water organisms	Photosynthetic suspression in Chlorella pyrenoidosa (as measured by 02 production via a modified Warburg apparatus) was 88% and 74%, as compared with the control, at concentrations of 100 and 500 mg/l, respectively. The concentration at which no substantial toxicity occurred was 10 mg/l. The tests were performed under steady-state conditions, algal density was 1.0 g/l (dry wt), 25 °C, aerated (with 5% CO2 in air) for a period of 72 hours with constant illumination (Sax 1986).	
Other information about water organisms	Tetrahymena pyriformis; EC50, grw, 67.97 mg/l, 2 days (Schultz 1987).	
Other information	More toxic than meta or para isomers (Sax 1986).	

525 • 3-Chlorophenol

108-43-0

Synonyms	m-Chlorophenol 1-Chloro-3-hydroxybenzene	
Sumformula of the chemical	C6H5OCl	
State and appearance	needles	
Molecular weight	128.56	
Vapour pressure, mmHg	5	72 °C
Water solubility, mg/l	29530 22420 > 800	25 °C (Cheug 1984) 20 °C (Mulley & Metcalf 1966) (MITI 1992)
Melting point, °C	33 30	(Doedens 1967) (MITI 1992)
Boiling point, °C	214	
pKa	8.85 8.52	(Doedens et al. 1967) (Ugland et al. 1981)
Log octanol/water coefficient, log Pow	2.5 2.47 2.27	(Fuita et al. 1966) (Hansch & Leo 1979) (Konemann & Musch 1981)
Aerobic degradation in soil	AEROBIC DEGRADATION IN SOIL Maximum adsorption wavelength: 275 nm NON-STERILE SOIL Minimum time for > 70% decrease: 80.0–160.0 d % decomposition at the termination of the experiment: 160d, 87% STERILE SOIL % decomposition at the termination of the experiment: 160d, 31% (Baker et al. 1980).	
Anaerobic degradation in soil	ANAEROBIC DEGRADATION IN SOIL Maximum adsorption wavelength: 275 nm NON-STERILE SOIL % decomposition at the termination of the experiment: 160d, 37% STERILE SOIL % decomposition at the termination of the experiment: 160d, 15% (Baker et al. 1980).	
Total degradation in soil	Decomposition rate in soil suspensions: > 72 days for complete disappearance (Verschueren 1983).	
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	5.1–10 7–16	6w, Cyprinus carpio, conc 0.04 mg/l 6w, Cyprinus carpio, conc 0.004 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	570	orl-rat (Lewis & Sweet 1984)

LD50 values to mammals in non-oral exposure, mg/kg	355 1390	ipr-rat scu-rat (Lewis & Sweet 1984)
LC50 values to fishes, mg/l	3 6.5 3.8	48hr, Leuciscus idus (Dietz & Traud 1978) 24hr, Poecilia reticulata (Könemann 1979) 48hr, Oryzias latipes (MITI 1992)

526 • 4-Chlorophenol

106-48-9

Synonyms	p-Chlorophenol 1-Chloro-4-hydroxybenzene	
Sumformula of the chemical	C6H5OCl	
Molecular weight	128.56	
Vapour pressure, mmHg	0.1	20 °C
Water solubility, mg/l	27100 27000 26500 < 800	20 °C 25 °C (Vesala 1974) 20 °C (Mulley & Metcalf 1966) (MITI 1992)
Melting point, °C	40–43	(MITI 1992)
Boiling point, °C	220	(MITI 1992)
pKa	9.18 9.37	(Doedens 1967) (Ugland et al. 1981)
Log octanol/water coefficient, log Pow	2.4 2.35 2.39 2.44 2.53	(Anon. 1986) (Hansch & Leo 1979) (Fiuta et al. 1964) (Hansch & Leo 1979) (Hansch & Leo 1979)
Henry's law constant, Pa x m³/mol	0.06285	calc. (Suntio et al. 1988)
Aerobic degradation in soil	AEROBIC DEGRADATION IN SOIL Maximum adsorption wavelength: 281 nm NON-STERILE SOIL Minimum time for > 70% decrease: 1.00–2.00 d % decomposition at the termination of the experiment: 20d, 83% STERILE SOIL % decomposition at the termination of the experiment: 20d, 5% (Baker et al. 1980).	
Anaerobic degradation in soil	ANAEROBIC DEGRADATION IN SOIL Maximum adsorption wavelength: 281 nm NON-STERILE SOIL % decomposition at the termination of the experiment: 40d, 13% STERILE SOIL % decomposition at the termination of the experiment: 40d, 17% (Baker et al. 1980).	
Total degradation in soil	Decomposition rate in soil suspensions: 9 days for complete disappearance (Verschueren 1983).	

Total degradation in water	Biodegradation: 2.0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	10 ppm	Carassius auratus (Verschueren 1983)
	6.0–18	6w, Cyprinus carpio, conc 0.04 mg/l
	11–52	6w, Cyprinus carpio, conc 0.004 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	261	orl-rat
	500	orl-mam (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	1000	skn-mam (Lewis & Sweet 19849
LD50 values to birds in oral exposure, mg/kg	> 113	orl-Agelaius phoeniceus (Schafer et al. 1983)
EC50 values to microorganism, mg/l	178	OECD 209 (Klecka et al. 1985)
LC50 values to crustaceans, mg/l	4.1	48hr, Daphnia magna (LeBlanc 1980)
	21	96hr, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	4.5	48hr, Leuciscus idus (Dietz & Traud 1978)
	3.8	96hr, Lepomis macrochirus (Buccafusco et al. 1981)
	5.4	96hr, Cyprinodon variegatus (Heitmuller et al. 1981)
	9	24hr, Carassius auratus (Kobayashi et al. 1979)
	1.9	96hr, Salmo gairdneri (Hodson et al. 1984)
	3.4	48hr, Oryzias latipes (MITI 1992)

527 • 4-Chlorophenoxyacetic acid 122-88-3

Synonyms	4-CPA	
Known impurities	Technical grade contains approximately 4% of 4-chloro-o-cresol.	
Use	Phytocide.	
Molecular weight	186	
Melting point, °C	157–159 °C	
Photochemical degradation in water	Primary products: 4-hydroxyphenoxyacetic acid, phenoxyacetic acid and p-chlorophenole (Verschueren 1983).	
Other information about degradation	Biodegradation: 11 days for ring cleavage in soil suspensions (Alexander 1972).	
LD50 values to birds in oral exposure	> 104	orl-Agelaius phoeniceus (Schafer et al. 1983)

Effects on plants	Root segments of aspen (Populus tremula) were treated with buffered solutions of 4-chlorophenoxy acetic acid for 24 hours: 0.0001 M (concentration of the solution) → strong inhibition of the shoot formation from aspen roots (Eliasson 1961). Aspen plants (Populus tremula) were grown in solutions: 0.000001 M (concentration of the solution) → swelling of the stem base, time of survival > 25 days; 0.00001 M → epinastic curvatures, swelling of the stem base, time of survival > 25 days (Eliasson 1963).
EC50 values to microorganism, mg/l	147.7 Microtox (Kaiser et al. 1985)
LC50 values to fishes, mg/l	147 24hr, Salmo trutta (Hattula et al. 1972)

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528 • 10-Chlorophenoxyarsine 2865-70-5

Other information about mammals	ALD = 42.0 mg/kg, act, orl, deer mouse; LDfr = 100 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

529 • 1-(p-Chlorophenyl)-3-(2,6-difluorobenzoyl)urea 35367-38-5

Synonyms	N-(((4-Chlorophenyl)amino)carbonyl)-2,6-difluorobenzamide Diflubenzuron Difluron Dimilin
Sumformula of the chemical	C14H9ClF2N2O2
Use	Insect growth regulator. Insecticide.
Molecular weight	310.7
Water solubility, mg/l	0.2
Melting point, °C	239
Log soil sorption coefficient, log Kom	3.83 (Sabljic 1987)
Hydrolysis in water	Hydrolyzes in water to p-chlorophenylurea (Verschueren 1983).
LD50 values to mammals in oral exposure, mg/kg	4640 orl-mus (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	2000 skn-rbt (Lewis & Sweet 1984)
Effects on arthropods	Aedes aegypti; LC50, > 0.00050 mg/l (Walker & Wood 1986) Aedes aegypti; LC50, 3 d, 0.00203 mg/l Aedes taeniorhynchus; LC50, 3 d, 0.00181 mg/l Anopheles albimanus; LC50, 3 d, 0.00142 mg/l Anopheles quadrimaculatus; LC50, 3 d, 0.00124 mg/l Chironomus crassicaudatus; LC50, 5 d, 0.00262 mg/l Culex nigripalpus; LC50, 3 d, 0.00111 mg/l Culex quinquefasciatus; LC50, 3 d, 0.00143 mg/l Culex salinarius; LC50, 3 d, 0.00292 mg/l (Ali & Nayar 1987)
LC50 values to crustaceans, mg/l	0.0021 96hr, Mysidopsis bahia (Nimmo et al. 1979)

LOEC values to crustaceans, mg/l	0.002	act, Daphnia magna
	0.002	act, Hyalella azteca
	0.0016	act, Chironomus spp. (Nebeker et al. 1983)b
	0.000075	rpd, achr, Mysidopsis bahia (Nimmo et al. 1979)
LC50 values to fishes, mg/l	370	96hr, Ictalurus punctatus
	250	96hr, Salmo gairdneri (Julin & Sanders 1978)
LOEC values to fishes, mg/l	> 0.036	srv, act, Pimephales promelas (Nebeker et al. 1983)
Other information	Inhibitor of syntesis of kitin (Verschueren 1983)	

530 • 4-Chlorophenyl acetic acid 1878-66-6

Synonyms	(4-Chlorophenyl)acetic acid	
EC50 values to microorganism, mg/l	64.6	Microtox (Kaiser et al. 1985)

531 • 4-Chlorophenyl isocyanate 104-12-1

Sumformula of the chemical	C7H4ClNO	
EC50 values to microorganism, mg/l	2.6	Microtox (Kaiser et al. 1985)

532 • 1-(p-Chlorophenyl)silatrane 29025-67-0

Other information about mammals	ALD = 8.0 mg/kg, act, orl, deer mouse; LDfr = 37.5 mg/kg, subacute, deer mouse (Virtanen & Nuuja 1987)

533 • 4-Chlorophenyl-3'-iodide-propargylformal 29772-02-9

Sumformula of the chemical	C10H8O2ClI	
Melting point, °C	14.5–16.5 (MITI 1992)	
Boiling point, °C	130	/0.2 mmHg (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

534 • 4-Chlorophenylphenyl sulfone 80-00-2

Synonyms	Sulphenone	
LD50 values to birds in oral exposure, mg/kg	> 100	orl-Agelaius phoeniceus
	> 100	orl-Passer domesticus (Schafer et al. 1983)

EC50 values to microorganism, mg/l	7.9	Microtox (Kaiser et al. 1985)

535 • 4-Chlorophenylurea 140-38-5

LC50 values to fishes, mg/l	72	96hr, Salmo gairdneri, Julin & Sanders 1978

536 • 6-Chloropicolinic acid 4684-94-0

Synonyms	Chloropicolinic acid
Sumformula of the chemical	C6H4O2NCl
Use	Sole metabolite other than carbon dioxide from degradation of 2-chloro-6-(trichloromethyl)pyridine.
Log soil sorption coefficient, log Kom	0.95 (Sabljic 1987)
Total degradation in soil	In soil at 1.0 ppm w initial conc. after 35 days incubation: *soil temperature °C* / *%-decomposition* 34–35 / 47.7 18–21 / 35.8 2–3 / 17.5 The most important factor influencing the decomposition rate is soil temperature (Meikle et al. 1976).

537 • Chloroprene 126-99-8

Synonyms	2-Chloro-1,3-butadiene β-Chloroprene
Sumformula of the chemical	C4H5Cl
Use	Manufacture of neoprene.
State and appearance	Colourless liquid.
Odour	Characteristic slightly etheric, threshold odour concentration recogn. 0.40 mg/m³ = 0.11 ppm (Leonardos et al. 1969)
Molecular weight	88.5
Specific gravity (water=1)	0.958 at 20 °C
Vapour density (air=1)	3.06
Conversion factor, 1 ppm in air=	3.68
Conversion factor, 1 mg/m³ in air=	0.27
Vapour pressure, mmHg	118 at 10 °C 200 at 20 °C 275 at 30 °C
Melting point, °C	-130
Boiling point, °C	59.4
Flashing point, °C	-20

Other physicochemical activities	Slightly soluble in water. Flammable, dangerous fire risk, explosive limits in air 4.0 to 20%. Toxic by ingestion, inhalation, and skin absorption.	
LD50 values to mammals in oral exposure, mg/kg	670	LD100 orl-rat (Patty 1967)
LC50 values to mammals in inhalation exposure, ppm	829 277	LD100 ihl-rat 1hr LD0 ihl-rat 1hr (Patty 1967)
Health effects	Man: loss of hair	

538 • 2-Chloropyridine 109-09-1

Water solubility, mg/l	20000	(MITI 1992)
Boiling point, °C	170	(MITI 1992)
Total degradation in water	Biodegradation: 0.5% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 1.9 < 19	6w, Cyprinus carpio, conc 1 mg/l 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LD50 values to birds in oral exposure, mg/kg	1000 > 1000 > 1000 > 1000	orl-Agelaius phoeniceus orl-Sturnus vulgaris orl-Coturnix coturnix orl-Passer domesticus (Schafer et al. 1983)
EC50 values to microorganism, mg/l	69.7	Microtox (Kaiser and Ribo 1985)
LC50 values to fishes, mg/l	880	48hr, Oryzias latipes (MITI 1992)
Other information about water organisms	Tetrahymena pyriformis; EC50, grw, 657.77 mg/l, 2.5d (Schultz et al. 1987).	

539 • 3-Chloropyridine 626-60-8

LD50 values to birds in oral exposure, mg/kg	1000 1000 750 562	orl-Agelaius phoeniceus orl-Sturnus vulgaris orl-Coturnix coturnix orl-Passer domesticus (Schafer et al. 1983)
EC50 values to microorganism, mg/l	66.5	Microtox (Kaiser and Ribo 1985)
Other information about water organisms	Tetrahymena pyriformis; EC50, grw, 619.68 mg/l, 2.5 d (Schultz et al. 1987).	

540 • 4-Chloropyridine HCl

7379-35-3

Use	Insecticide.
LD50 values to birds in oral exposure, mg/kg	100–1000 orl-Agelaius phoeniceus > 1000 orl-Sturnus vulgaris > 1000 orl-Coturnix coturnix > 1000 orl-Passer domesticus (Schafer et al. 1983)

541 • Chlorothalonil

1897-45-6

Synonyms	Tetrachloroisophthalonitrile
Use	Fungicide.
State and appearance	White chrystalline solid.
Water solubility, mg/l	0.6
Melting point, °C	251
Half-life in soil, days	70 (Li et al. 1990)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.1–2.7 6w, Cyprinus carpio, conc 0.03 mg/l < 1.3–125 6w, Cyprinus carpio, conc 0.003 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	> 10000 orl-rat (Anon. 1976)
LD50 values to mammals in non-oral exposure, mg/kg	> 10000 idr-rat, Anon.1976
Carcinogenicity	It is concluded that under the conditions of this bioassay, technical-grade chlorothalonil was carcinogenic to Osborne-Mendel rats, producing tumors of the kidney. Chlorothalonil was not carcinogenic for B6C3F1 mice (Verschueren 1983).
LC50 values to crustaceans, mg/l	7.8 act, Daphnia pulex (Hashimoto & Nishiuchi 1981) 7.8 act, Daphnia pulex (Nishiuchi & Hashimoto 1967)
LC50 values to fishes, mg/l	0.25 act, Salmo gairdneri (Pesticide Manual 1983) 0.17 48hr, Carassius auratus 0.11 48hr, Cyprinus carpio (Hashimoto & Nishiuchi 1981) 0.11 48hr, Cyprinus carpio (Nishiuchi & Hashimoto 1967) 0.28 48hr, Oryzias latipes (MITI 1992)

542 • 2-Chlorotoluene

95-49-8

Synonyms	o-Chlorotoluene 2-Chloro-1-methylbenzene

Sumformula of the chemical	C7H7Cl	
Use	Solvent and intermediate for organic chemicals and dyes.	
Molecular weight	126.58	
Melting point, °C	-36.5	
Boiling point, °C	159	760 mmHg (MITI 1992)
Specific gravity (water=1)	1.0817	at 20/4 °C
Vapour density (air=1)	4.37	
Conversion factor, 1 ppm in air=	5.26	
Conversion factor, 1 mg/m³ in air=	0.19	
Vapour pressure, mmHg	2.7 5	at 20 °C at 30 °C
Log octanol/water coefficient, log Pow	3.42 3.42	(Anon. 1988) (Sangster 1989)
Henry's law constant, Pa x m³/mol	780	(Anon. 1988)
Mobility	Equilibrium distribution: air water solid	 *mass %* 99.48 0.37 0.15 (Anon. 1988).
Total degradation in water	Biodegradation: 0% by BOD period: 28w substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	41.6–87.2 20–112	8w, Cyprinus carpio, conc 0.45 mg/l 8w, Cyprinus carpio, conc 0.045 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 15 mg/l (Bringmann & Kühn 1980a).	
LC50 values to fishes, mg/l	9.6	48hr, Oryzias latipes (MITI 1992)
Effects on the reproduction of water organisms	Cell pultiplication inhibition test: Pseudomonas putida 15 mg/l Scenedesmus quadricauda> 100 mg/l (Bringmann & Kühn 1980a) Entosiphon sulcatum> 80 mg/l Uronema parduczi Chatton-Lwoff > 80 mg/l (Bringmann & Kuhn 1980b)	
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): > 100 mg/l protozoa (Entosiphon sulcatum): > 80 mg/l (Bringmann & Kühn 1980a).	

543 • 3-Chlorotoluene 108-41-8

Sumformula of the chemical	C7H7Cl	
Log octanol/water coefficient, log Pow	3.28	(Sangster 1989)
LC50 values to fishes, mg/l	18	7 d, Poecilia reticulata (Könemann 1979)

544 • 4-Chlorotoluene 106-43-4

Synonyms	p-Chlorotoluene	
Sumformula of the chemical	C7H7Cl	
Use	Solvent and intermediate for organic chemicals and dyes.	
Molecular weight	126.59	
Specific gravity (water=1)	1.066	25/15 °C
Boiling point, °C	162–166 161.99	 (MITI 1992)
Log octanol/water coefficient, log Pow	3.33	(Sangster 1989)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	21.9–76.5 14–101.6	8w, Cyprinus carpio, conc 0.3 mg/l 8w, Cyprinus carpio, conc 0.03 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	3600 1900	orl-rat orl-mus (Lewis & Sweet 1984)
LC50 values to mammals in inhalation exposure, mg/m³	34000	2hr, ihl-mus (Lewis & Sweet 1984)
EC50 values to microorganism, mg/l	4.9	Microtox (Kaiser et al. 1985)
LC50 values to crustaceans, mg/l	1.6	srv, schr, 16 d, Daphnia magna (Hermens et al. 1984)
EC50 values to crustaceans, mg/l	0.58	rpd, schr, 16 d, Daphnia magna (Hermens et al. 1984)
NOEC values to crustaceans, mg/l	1 0.32	srv, schr, 16 d, Daphnia magna (Hermens et al. 1984) rpd, schr, 16 d, Daphnia magna (Hermens et al. 1984)
LC50 values to fishes, mg/l	5.9 5.2	14 d, Poecilia reticulata (Könemann 1979) 48hr, Oryzias latipes (MITI 1992)

545 • Chlorotriphenylmethane 76-83-5

Water solubility, mg/l	< 10 (MITI 1992)
Melting point, °C	112–113 (MITI 1992)
Log octanol/water coefficient, log Pow	5.25 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	206–374 8w, Cyprinus caarpio, conc 0.5 mg/l 215–649 8w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	197 48hr, Oryzias latipes (MITI 1992)

546 • Chloroxuron 1982-47-4

Synonyms	Tenoran 3-(p-(p-Chlorophenoxy)phenyl)-1,1-dimethylurea
Use	Active ingredient in herbicides. Absorbed by both roots and leaves.
State and appearance	White crystals.
Melting point, °C	149–150
LD50 values to mammals in oral exposure, mg/kg	3700 orl-rat > 100000 orl-rbt
LC50 values to fishes, mg/l	25 48hr, Lepomis macrochirus (Hughes & Davis 1964)

547 • Chlorphenamidine 6164-98-3

Synonyms	Chlordimeform N'-(4-Chloro-o-tolyl)-N,N-dimethylformamidine Chlorfenamide N'-(4-Chloro-2-methylphenyl)-N,N-dimethylmethanimidamide Chlorophenamidine N,N-Dimethyl-N'-(2-methyl-4-chlorophenyl)formamidine
Sumformula of the chemical	C10H13ClN2
Use	Broad spectrum insecticide which is effective for all stages of insects and mites including eggs and adults. Chlorphenamidine hydrochloride has been used for the control of the rice stem borer in Japan.
State and appearance	Buff coloured crystals.
Molecular weight	196.7
Melting point, °C	32
Metabolism in plants	The major metabolites by plants are: N'-(4-chloro-o-tolyl)N-methylformamidine (desmethylchlorphenamidine); N-formyl-4-chloro-o-toluidine; 4-chloro-o-toluidine (Verschueren 1983).

LD50 values to mammals in oral exposure, mg/kg	127–352	tech. grade orl-rat (Verschueren 1983)
	160	orl-mus, orl-rat
	625	orl-rbt (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	> 3000	skn-rbt (Verschueren 1983)
	86	ipr-mus
	90	ipr-rat
	225	skn-mus
	263	skn-rat
	640	skn-rbt (Sweet 1987)
TDLo values to mammals in oral exposure, mg/kg	6552	orl-mus, tumorigenic
	1.8	orl-rat, 5–22d preg. effects on newborn (Sweet 1987)

548 • Chlorphoxim

14816-20-7

Synonyms	2-Chloro-α-(((diethoxyphosphinothioyl)oxy)imino)benzeneacetonitrile (o-Chlorophenyl)glyoxylonitrileoxime-0,0-diethylphosphorothioate
Use	Pesticide. Effective against the larval stages of Simulium damnosum (blackfly), the insect vector of human onchocerciasis in Africa; effective against adult mosquitoes and agricultural insects.
Bioconcentration factor, fishes	150 (Zakitis 1979)

549 • Chlorpropham

101-21-3

Synonyms	Isopropyl-N-(3-chlorophenyl)carbamate	
Use	Active ingredient in herbicides.	
LD50 values to birds in oral exposure, mg/kg	> 500	orl-Agelaius phoenicus
	> 500	orl-Sturnus vulgaris (Schafer et al. 1983)
LC50 values to fishes, mg/l	8	48hr, Lepomis macrochirus (Hughes & Davis 1964)

550 • Chlorsulfuron

64902-72-3

Sumformula of the chemical	C12H12ClN5O4S
Products containing the chemical	Glean 20 DF * chlorsulfuron 200 g/kg (PESREG)
Use	Active ingredient in herbicides.
State and appearance	Solid, crystalline, white. (PESREG)
Odour	Odourless. (PESREG)
Molecular weight	357.78
Vapour pressure, mmHg	0.0000046 at 25 °C (PESREG) 0.0000045 at 25 °C (KEMI 1990)

Water solubility, mg/l	125 at 25 °C (PESREG) 27900 at 25 °C, pH 7 (KEMI 1990)
Melting point, °C	174 (PESREG) 174–178 °C (KEMI 1990)
Degradation point, °C	192 (PESREG)
pKa	3.8 (KEMI 1990)
Log octanol/water coefficient, log Pow	1.11 at 24–26 °C (PESREG) 0.48 (KEMI 1990)
Mobility	The mobility of chlorsulfuron was studied with six different soils under field conditions in the natural rainfall. *% C-14activity after 52 weeks in 10–20 cm soil depth* 15.0% loam, C-14-phenyl-labelled 20.2% silt loam, C-14-phenyl-labelled 10.5% silt loam, C-14-triazine-labelled 15.6% silt loam, C-14-phenyl-labelled 10.6% silt loam, C-14-phenyl-labelled 22.7% sandy loam, C-14-phenyl-labelled 6.0% silty clay loam, C-14-phenyl-labelled (PESREG) The leaching behaviour of chlorsulfuron was studied in fo ur different soil (sandy loam, two silt loam and sandy soils) columns. When chlorsulfuron was applied and immediately leached from 76 to 83% of applied radioactivity percolated through the columns with 20 inches of water within 20 hours. When it was used aged soil columns (aged 30 days) 20 to 33% of applied radioactivity leached from these columns. (PESREG) The mobility of chlorsulfuron in soil is very high first of all in soils with high pH and low organic material. Ka: 0.45–0.69. (KEMI 1990) Solubility in organic solvents: *wt/wt* *wt/vol* hexane 10 ppm toluene 0.3% 0.3% methanol 1.8% 1.4% acetone 7.0% 5.7% methylene chloride 7.7% 10.2% N,N-dimethylformamide 27.3% 27.4% (PESREG)
Photochemical degradation in soil	The photodegradation of chlorsulfuron was studied in two soils (sandy loam and silt loam) with simulated sunlight at 45 °C in the laboratory. The half-life was about two weeks in both soils. The major product was 2-chlorobenzenesulfonamide (from C-14-phenyl-labelled) and this compound increased to 30–35% of the residual radioactivity after 4 weeks of photolysis. (PESREG) Photolysis on surface of soil is not significant. (KEMI 1990)
Photochemical degradation in water	The photodegradation of chlorsulfuron (1 and 10 ppm) in aqueous solutions was studied in the laboratory using a fluorescent light source. 10% of the intact compound remained after 4 weeks' exposure. The major decomposition products were 2-chlorobenzenesulfonamide and 2-amino-4-methoxy-6-methyl-1,3,5-triazine. (PESREG)

Hydrolysis in water	The hydrolysis of chlorsulfuron was studied at pH 7 and pH 9. Chlorsulfuron was stable for at least 4 weeks. (PESREG) Hyrdolysis of chlorsulfuron is strongly dependent on pH and varies between temperatures, too. The half-life at pH 4 is 1 week at 20 °C and 10–14 days at 10 °C. In neutral and basic coditions hydrolysis is more slowly. (KEMI 1990) At hydrolysis chlorsulfuron devides into two spieces; 2-chlorobenzenesulfonamide and 2-amino-4-methoxy-6-methyl-1,3,5-triazine. The last one degrades very slowly. (KEMI 1990)
Hydrolysis in acid	The half-life of chlorsulfuron (1-10 ppm) were one week (20 °C) and 10–14 days (10 °C). The hydrolysis product (C-14-phenyl-labelled) was 2-chlorobenzene-sulfonamide. The hydrolysis product (C-14-triazine-labelled) was first 2-amino-4-methoxy-6-methyl-1,3,5-triazine and then it by stepwise loss of the methoxy and amino groups and 2,4-dihydroxy-6-methyl-1,3,5-triazine formed. (PESREG)
Aerobic degradation in soil	The half-life of chlorsulfuron (C-14-phenyl labelled) under aerobic conditions in a greenhouse was about 2 month (in sandy loam and silt loam). The major degradation product in both soils was 2-chlorobenzenesulfonamide increasing to 30–35% of the residual radioactivity after 3 months and then slowly declining to 12–13% after 9 months. (PESREG)
Anaerobic degradation in sediment	The half-life of chlorsulfuron was 7 to 8 weeks in anaerobic flooded soil (soil and distilled deionized water) system. The degradationproducts were 2-chlorobenzenesulfonamide and 2-chlorophenylsulfonylurea (from C-14-phenyl-labelled). (PESREG)
Total degradation in soil	The half-life of chlorsulfuron in soil (three sandy loams and three silt loams) under field conditions was about 1 month (in the acidic soils). In the alkaline soil the half-life was 2–3 months. The major degradation product was 2-chlorobenzenesulfonamide (from C-14-phenyl-labelled) and 2-amino-4-methoxy-6-methyl-1,3,5-triazine (from C-14-triazine-labelled). (PESREG) The biodegradation of chlorsulfuron was studied in sterile and nonsterile silt loam soils. *14CO2 amount (%) after 7 weeks* *C-14-phenyl-labelled* / *C-14-triazine-labelled* sterile soil: 0.5 / 2.5 nonsterile soil: 5 / 23 degradation product: 2-chlorobenzene-2-amino-4-methoxy- sulfonamide 6 methyl-1,3,5-triazine The half-life was between one and two weeks. (PESREG)
Degradation and transformation products	C-14-phenyl-labelled: 2-chlorobenzenesulfonamide C-14-triazine-labelled: 2-amino-4-methoxy-6-methyl-1,3,5-triazine 2,4-dihydroxy-6-methyl-1,3,5-triazine
Other information about degradation	The hydrolysisproducts of chlorsulfuron is degraded by microorganisms. Degradation is very slow. The half-life in the field may be many months. In the laboratory the half-life is obviously shorter, about 1–2 weeks at 25 °C. (KEMI 1990)
LD50 values to mammals in oral exposure, mg/kg	5545–6293 orl-rat, KEMI 1990
LD50 values to mammals in non-oral exposure, mg/kg	> 3400 idr-rbt (KEMI 1990)
LC50 values to mammals in inhalation exposure, mg/m³	> 5900 ihl-rat (KEMI 1990)

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LD50 values to birds in oral exposure, mg/kg	> 5000 orl-Anas platyrhyncos > 5000 orl-Coturnix virginianus (PESREG) > 5000 orl-Anas platyrhynchos > 5000 orl-Coturnix virginianus (KEMI 1990)
Subacute LC50 values to birds in feeding exposure, mg kg	> 5000 5d+3d, Anas platyrhyncos > 5000 5d+3d, Coturnix virginianus (PESREG) > 5000 8d, Anas platyrhyncos > 5000 8d, Coturnix virginianus (KEMI 1990)
Effects on bees	LD50 (24hr) > 20 µg/bee, Glean * (KEMI 1990)
Effects on microorganisms	There was no effect with chlorsulfuron (0.1 and 1.0 ppm, 35 °C, 10 weeks) tratment on the soil nitrification (silt loam soil and sandy loam soil). (PESREG) Chlorsulfuron has no effect to the nitrification process in soil. (KEMI 1990)
EC50 values to algae, mg/l	4.3 96hr, Chlorella vulgaris 1.2–2.5 72hr, Selenastrum capricornutum 0.016 120hr, Synechococcus leopoliensis (KEMI 1990)
NOEC values to algae, mg/l	1 Chlorella vulgaris (KEMI 1990) 0.5 Selenastrum capricornutum (KEMI 1990) 0.0036 Synechococcus leopoliensis (KEMI 1990)
LC50 values to crustaceans, mg/l	370.9 48hr, Daphnia magna (PESREG) 370 48hr, Daphnia magna (KEMI 1990)
EC50 values to crustaceans, mg/l	> 480 21d, imb, Daphnia magna > 480 21d, rpd, Daphnia magna GLP, OECD No 202 (PESREG)
LOEC values to crustaceans, mg/l	120 21d, srv, young Daphnia magna 28 21d, grw, Daphnia magna GLP, OECD No 202 (PESREG)
NOEC values to crustaceans, mg/l	58 21d, srv, young Daphnia magna 12 21d, grw, Daphnia magna GLP, OECD (PESREG) 20 NOEL, 21d, rpd, Daphnia magna GLP, OECD (PESREG)
LC50 values to fishes, mg/l	> 250 96hr, Salmo gairdneri Lepomis macrochirus (Pesticide Manual 1983) > 50 96hr, Ictalurus punctatus > 300 96hr, Pimephales promelas > 300 96hr, Lepomis macrochirus > 300 96hr, Salmo gairdneri (PESREG) 250–300 96hr, Salmo gairdneri (KEMI 1990)
Other information about water organisms	NOEC: 0.00004 mg/l Lemna minor. EC50 (14d): 0.00011 mg/l Lemna minor. (KEMI 1990)

551 • Chlorthiamid

1918-13-4

Synonyms	2,6-Dichloro(thiobenzamide)	
Use	Active ingredient in herbicides.	
LC50 values to fishes, mg/l	41	24hr, Rasbora heteromorpha (Alabaster 1969)

552 • Chlorthion

500-28-7

Use	Insecticide.	
LD50 values to birds in oral exposure, mg/kg	> 280 > 500 > 100	orl-Agelaius phoeniceus orl-Sturnus vulgaris orl-Passer domesticus (Schafer et al. 1983)
LC50 values to crustaceans, mg/l	0.0045	48hr, Daphnia magna (Pickering et al. 1962)
LC50 values to fishes, mg/l	0.7 2.8	96hr, Lepomis macrochirus 96hr, Pimephales promelas (Pickering et al. 1962)

553 • Chlortoluron

15545-48-9

Use	Herbicide.
Effects on plants	0.125 kg a.i. chlortoluron/ha was applied with a sprayer to blackgrass (Alopecurus myosuroides Huds.) at the 2 to 3-leaf stage —a decrease in mean fresh weight of plants (Blair 1978).

554 • Chromium(3+) compounds

16065-83-1

Sumformula of the chemical	Cr	
Molecular weight	52	
Mobility	Chromium is normally in three (as kation) or six (as anion) valent forms in soil and water. In soil Cr3+ is precipitated even in acid environment (pH 5,5). CrVI compounds are unstable both in acid and alkaline soils. With precense of organic matter CrVI reduces to Cr3+ (Kabata-Pendias & Pendias 1984). In water CrVI is often dominating the soluble fraction as well in oceans and in running water. Cr3+ dominates when organic matter is available. CrVI is therefore rare in municipal effluents (Balsberg-Påhlsson et al. 1982).	
Metabolism in mammals	Metabolism in mammals is not quite clear (USEPA 1985). Experiments with animals has shown that that Cr3+ salts are not easily absorped in oral intake. Excretes mostly with urine (Kraintz & Talmage 1952).	
Other information about bioaccumulation	Cr in fish concentrates in gills, kidneys, liver, gall and spleen (Balsberg-Påhlsson et al. 1982). CrVI is taken up easier than Cr3+. In cells CrVI is reduced to Cr3+ (Taylor et al. 1979). Cr taken up with food is more important than Cr taken up with water to all aquatic animals except crustacean and fry. Accumulation decreases with growing trophic level (Baptist & Lewis 1969).	
LD50 values to mammals in oral exposure, mg/kg	1870 600–2600	orl-rat, CrCl3 (Christensen 1973) orl-unk, Cr3+ (Smyth et al. 1969)

Other information about mammals	CrVI has most extended harmful effects. Exposure at low levels in mammals has induced effects in respiratory tract, such as bronchitis, pneumonia and tumours (WHO 1988). Rat, inhalation 28 d / 90d, changes in lungs: 0.006–0.2 mg/m³ (Glaser et al. 1985).
Carcinogenicity	Cr3+ considered not carcinogenic. CrVI salts are carcinogenic in epidemiologic tests (WHO 1988). Cr och certain Cr compounds, exposure via inhalation: Group 1, adequate proof for carcinogenicity to mammals and humans (IARC 1982); EPA Guidelines – group A, carcinogenic to humans (USEPA 1986).
Mutagenicity	Negative for Cr3+ (WHO 1988). CrVI salts are mutagenic to mammals in vivo and in vitro (WHO 1988).
Effects on plants	Two cultivars of cotton (Gossypium spp.) were grown in solution culture. The 0.0001 M Cr2(SO4)3 resulted in leaf yield reduction of 83% (0.022 mg Cr/g in leaf, 0.015 mg Cr/g in stem) and 88% (0.019 mg Cr/g in leaf) (Rehab & Wallace 1978c).
LC50 values to crustaceans, mg/l	2 — 21d, Daphnia magna, Cr3+ (Biesinger & Christensen 1972) 442 — 96hr, mbt, Asellus aquaticus 937 — 48hr, mbt, Asellus aquaticus (Martin & Holdich 1986)
EC50 values to crustaceans, mg/l	0.6 — 21d, rpd, Daphnia magna (Biesinger & Christensen 1972)
LOEC values to crustaceans, mg/l	0.33 — rpd, 21d, Daphnia magna (Biesinger & Christensen 1972) 0.5 — Palaemonetes pugio, Cr3+ (Doughtie & Rao 1984)
LC50 values to fishes, mg/l	4.4 — 96hr, Salmo gairdneri (Stevens & Chapman 1984) 58.5 — 96hr, Branchydanio rerio (Bellavere & Gorbi 1981)
LOEC values to fishes, mg/l	0.089 — srv, schr, Salmo gairdneri, Cr3+ (Stevens & Chapman 1984)
Other information about water organisms	EC0, Chlorella sp., 0.5 mg/l, Cr3+ (Nollendorf et al. 1972). Salmo salar, rpd, 0.1–1 mg/l, Cr3+ (Brånin & Paulsson 1971).

555 • Chromium and chromium compounds 7440-47-3

Sumformula of the chemical	Cr
Molecular weight	52
Mobility	Chromium is normally in three (as kation) or six (as anion) valent forms in soil and water. In soil Cr3+ is precipitated even in acid environment (pH 5,5). CrVI compounds are unstable both in acid and alkaline soils. With precense of organic matter CrVI reduces to Cr3+ (Kabata-Pendias & Pendias 1984). In water CrVI is often dominating the soluble fraction as well in oceans and in running water. Cr3+ dominates when organic matter is available. CrVI is therefore rare in municipal effluents (Balsberg-P}hlsson et al. 1982).
Metabolism in mammals	Metabolism in mammals is not quite clear (USEPA 1985). Experiments with animals has shown that that Cr3+ salts are not easily absorped in oral intake. Excretes mostly with urine (Kraintz & Talmage 1952).
Other information about bioaccumulation	Cr in fish concentrates in gills, kidneys, liver, gall and spleen (Balsberg-Påhlsson et al. 1982). CrVI is taken up easier than Cr3+. In cells CrVI is reduced to Cr3+ (Taylor et al. 1979). Cr taken up with food is more important than Cr taken up with water to all aquatic animals except crustacean and fry. Accumulation decreases with growing trophic level (Baptist & Lewis 1969).

Other information about mammals	CrVI has most extended harmful effects. Exposure at low levels in mammals has induced effects in respiratory tract, such as bronchitis, pneumonia and tumours (WHO 1988). Rat, inhalation 28 d / 90d, changes in lungs: 0.006–0.2 mg/m³ (Glaser et al. 1985).
Carcinogenicity	Cr3+ considered not carcinogenic. CrVI salts are carcinogenic in epidemiologic tests (WHO 1988). Cr och certain Cr compounds, exposure via inhalation: Group 1, adequate proof for carcinogenicity to mammals and humans (IARC 1982); EPA Guidelines – group A, carcinogenic to humans (USEPA 1986).
Mutagenicity	Negative for Cr3+ (WHO 1988). CrVI salts are mutagenic to mammals in vivo and in vitro (WHO 1988).
Teratogenicity	No teratogenic effects in humans have been indicated (WHO 1988)

556 • Chromium chloride 10025-73-7

EC50 values to crustaceans, mg/l	937	2d, mbt, Asellus aquaticus
	442	4d, mbt, Asellus aquaticus
	388	2d, mbt, Crangonyx pseudogracilis
	291	4d, mbt, Crangonyx pseudogracilis
		(Martin & Holdich 1986)

557 • Chromium(VI) compounds 18540-29-9

Sumformula of the chemical	Cr
Molecular weight	52
Mobility	Chromium is normally in three (as kation) or six (as anion) valent forms in soil and water. In soil Cr3+ is precipitated even in acid environment (pH 5,5). CrVI compounds are unstable both in acid and alkaline soils. With precense of organic matter CrVI reduces to Cr3+ (Kabata-Pendias & Pendias 1984). In water CrVI is often dominating the soluble fraction as well in oceans and in running water. Cr3+ dominates when organic matter is available. CrVI is therefore rare in municipal effluents (Balsberg-Påhlsson et al. 1982).
Metabolism in mammals	Metabolism in mammals is not quite clear (USEPA 1985). Experiments with animals has shown that that Cr3+ salts are not easily absorped in oral intake. Excretes mostly with urine (Kraintz & Talmage 1952).
Other information about bioaccumulation	Cr in fish concentrates in gills, kidneys, liver, gall and spleen (Balsberg-Påhlsson et al. 1982). CrVI is taken up easier than Cr3+. In cells CrVI is reduced to Cr3+ (Taylor et al. 1979). Cr taken up with food is more important than Cr taken up with water to all aquatic animals except crustacean and fry. Accumulation decreases with growing trophic level (Baptist & Lewis 1969).
LD50 values to mammals in oral exposure, mg/kg	19.8 orl-rat, CrVI (NIOSH 1983)
Other information about mammals	CrVI has most extended harmful effects. Exposure at low levels in mammals has induced effects in respiratory tract, such as bronchitis, pneumonia and tumours (WHO 1988). Rat, inhalation 28 d / 90d, changes in lungs: 0.006–0.2 mg/m³ (Glaser et al. 1985).

Carcinogenicity	Cr^{3+} considered not carcinogenic. CrVI salts are carcinogenic in epidemiologic tests (WHO 1988). Cr och certain Cr compounds, exposure via inhalation: Group 1, adequate proof for carcinogenicity to mammals and humans (IARC 1982); EPA Guidelines – group A, carcinogenic to humans (USEPA 1986).
Mutagenicity	Negative for Cr^{3+} (WHO 1988). CrVI salts are mutagenic to mammals in vivo and in vitro (WHO 1988).
Teratogenicity	No teratogenic effects in humans have been indicated (WHO 1988).
LC50 values to crustaceans, mg/l	1.84 96hr, Macrobrachium lamarrei, CrVI (Murti et al. 1983) 0.02 48hr, Daphnia pulex, CrVI (Dorn et al. 1987)
LOEC values to crustaceans, mg/l	0.0017 14d, Daphnia magna, CrVI (Elnabarawy et al. 1986)
LC50 values to fishes, mg/l	0.19 28d, Salmo gairdneri, CrVI (Birge et al. 1980) 200 96hr, Mystus vittatus (Verma et al. 1982) 36.2 96hr, Pimephales promelas (Pickering 1980) 45.2 96hr, Colisa fasciata (Saxena & Parashari 1983) 4.4 96hr, Salmo gairdneri, CrVI (Steven & Chapman 1989) 3.4 96hr, Salmo gairdneri, CrVI (van der Putte et al. 1981) 0.27–2.0 chr, Salmo gairdneri (USEPA 1980)
LOEC values to fishes, mg/l	0.025 grw, schr, Salmo gairdneri, CrVI (Olson & Forster 1956) 0.351 srv, grw, chr, Salvelinus fontinalis 0.34 srv, grw, schr, Salmo gairdneri (Benoit et al. 1976) 0.044 grw, schr, Oncorhynchus tschawytscha (Olson & Forster 1956) 3.95 srv, grw, chr, Pimephales promelas (Pickering 1980)
NOEC values to fishes, mg/l	0.021 grw, schr, Salmo gairdneri (Olson & Forster 1956) 0.2 srv, grw, schr, Salmo gairdneri (Benoit et al. 1976) 0.022 grw, schr, Oncorhynchus tschawytscha (Olson & Forster 1956) 1 srv, grw, chr, Pimephales promelas (Pickering 1980)
Effects on the physiology of water organisms	Selenastrum capricornutum; 0.020 mg/l, 0.17d, pht (Pillard et al. 1987).
Other information about water organisms	LOEC 0.5 mg/l, his, schr, Palaemonetes pugio (Doughtie & Rao 1984). Chlorella pyrenoidosa, effects on growth, 0.05 mg/l (CrVI) (Frey et al. 1983). Neanthes arenaceodentata, rpd, 350 days, < 0.012 mg/l CrVI (Mearns et al. 1976). Daphnia, rpd, 0.01 mg/l, CrVI (EIFAC 1983).

558 • Chromium(VI) oxide 1333-82-0

Synonyms	Chromic acid Chromic anhydride Chromic trioxide Chromic(VI) acid Chromium oxide Chromium trioxide Chromium (VI) oxide Monochromium oxide Monochromium trioxide

Sumformula of the chemical	CrO3	
Molecular weight	100	
Water solubility, mg/l	617000	0 °C
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	80 127	orl-rat orl-mus (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	29 14	ipr-mus (Lewis & Sweet 1984) ipr-mus (Sweet 1987)
LDLo values to mammals in non-oral exposure, mg/kg	330 20	scu-dog scu-mus (Sweet 1987)
TDLo values to mammals in non-oral exposure, mg/kg	5	ivn-ham, 8 d preg. specific developmental abnormalities
	7.5	ivn-ham, 8 d preg. effects on fertility effects on embryo of fetus specific developmental abnormalities
	8	ivn-ham, 8 d preg. specific developmental abnormalities
	20	scu-mus, 8 d preg. effects on embryos or fetus (Sweet 1987)
	125	implant-rat, tumorigenic (Sweet 1987)
TCLo values to mammals in inhalation exposure, mg/kg	0.11	ihl, hmn, tumorigenic (Sweet 1987)
Carcinogenicity	Inhalation: human TCLo 0.110 mg/m³/3Y-C; tumorigenic (carcinogenic by RTECS criteria); sense organs and special senses. Implant: rat TDLo 125 mg/kg; tumorigenic (carcinogenic by RTECS criteria); tumors at site of application.	
Mutagenicity	Mutation data: cyt, ham, emb, 0.068 mg/l; cyt, ham, ovr, 0.250 mg/l; cyt, ham, leu, 2 mg/l; cyt, mus, mmr, 1 µmol/l, 48hr; dnd, esc, 5 mmol/l; dnr, bsc, 50 mmol/l; dnr, sat, 50 mmol/l; microbial mutation without S9: esc, 8 µmol/l; sat, 1 mmol/l; mma, sat, 0.010 mg/plate; sce, ham, ovr, 0.250 mg/l; sce, ham, fbr, 0.320 mg/l (Sweet 1987).	
LC50 values to fishes, mg/l	40	96hr, Channa punctatus (Srivastava et al. 1979)

559 • Chrysene

218-01-9

Synonyms	1,2-Benzophenanthrene 1,2-Benz(a)phenanthrene 1,2,5,6-Dibenzonaphthalene
Sumformula of the chemical	C18H12

Use	Chrysene is used in organic synthesis. Chrysene occurs in coal tar and is formed during distillation of coal and in very small amounts during distillation or pyrolysis of many fats and oils. It is also found in exhaust grom gasoline and diesel engines, the atmosphere, soil, water, cigarette smoke, petroleum products, wood smoke, and foods.	
State and appearance	Crystals. Red, blue, fluorescent.	
Odour	Odourless.	
Molecular weight	228.2	
Specific gravity (water=1)	1.274	20/4 °C
Conversion factor, 1 ppm in air=	5.493	mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.182	ppm
Water solubility, mg/l	0.017 0.002 0.0015	24 °C 15 °C
Melting point, °C	254	
Boiling point, °C	448	
Log octanol/water coefficient, log Pow	5.61 5.86	 (Sangster 1989)
Other physicochemical properties	Insoluble in water. Soluble in ethanol at 0.097 parts chrysene / 100 parts ethanol at 16 °C, and 0.17 / 100 parts ethanol at 78 °C. 100 parts toluene dissolves 0.24 parts chrysene at 18 °C, and 5.39 parts chrysene at 100 °C. Sparingly soluble in glacial acetic acid, ether and carbon disulfide and slightly soluble in hot benzene or xylene. Sublimes easily in a vacuum. A partition coefficient for chrysene was determined between the two solvent phased hexane and aqueous monoethanolammonium desoxycholate to be 10.4 (Sax 1986).	
Photochemical degradation in air	Airborne particulate polycyclic aromatic hydrocarbons can persist at relatively high concentrations in aerosols transported for long distances. The atmosperic persistence is longer than would be predicted from laboratory photooxidation studies. On the other hand, the National Academy of Sciences (1972) proposed that the chemical half-life of PAHs in the atmosphere may be limited to hours or days (Sax 1986).	
Other chemical degradation processes	Ozone and chlorinating agents oxidize polycyclic aromatic hydrocarbons to quinones, diacids, and nuclear and side-chain oxidation products. Chlorinating agents also produce chlorine-substituted derivatives. – The most common photooxidation product in solution is an endo peroxide. Dealkylation, ring cleavage, and other reactions ensue following photolysis or pyrolysis of these peroxides. Frequently, only quinones are isolable. Photodimers may result in some cases. Absorbed PAH's are more reactive than in solution (Sax 1986).	
Total degradation in sediment	PAHs deposited in sediments are less subject to photochemical or biological oxidation, especially if the sediment is anoxic. Sedimentary PAH is therefore quite persistent and may accumulate to high concentrations (Sax 1986).	

Other information about degradation	Biodegradation may be less slow in the soil than in aquatic systems. – Oxidation of any PAH by chlorine and ozone, when used for the disinfection of drinking water, forms quinones. – Chlorinating agents will also produce chlorine-substituted PAHs as well as oxidation products. – The half-life for the reaction of all PAHs with chlorine is less than 0.5 hour. – Hydrolysis is not significant. Photolysis in an aquatic environment may be an important fate process, especially for the dissolved portion. The half-life for chrysene photolysis calculated for surface waters in midsummer at 40 degrees north latitude was 4.4hr. – Evaporation of lower-molecular-weith PAHs may be significant only in a clear, rapidly flowing shallow stream. – Movement via sediment is considered to be an important transport process for PAHs. An exchange equilibrium exists in natural water systems between absorbed and soluble PAHs. Although the particulate form if favored, a significant fraction of the PAH will be dissolved except in systems that are very heavily contaminated by PAHs. – However, chrysene was found to be more resistant to microbial degradation than 6 other PAHs having 3 to 5 aromatic rings. – The concentrations of bacteria and fungi capable of oxidizing hydrocarbons are extremely low in all but heavily polluted fresh and marine waters. Most species cannot use PAHs as a sole carbon source. Microbial oxidation of PAHs requires oxygen and will not proceed in anoxic sediments or water (Sax 1986).
Other information about metabolism	There are large differences among species in their ability to absorb and assimilate PAHs from food. Polychaete worms have a very limited ability, fish show limited and variable absorption from the gut, and crustaceans readily assilimate PAHs. Assimilated PAHs are metabolized and excreted rapidly. For biomagnification to occur, a substance must be relatively resistant to metabolism or exreation (Sax 1986).
Other information about bioaccumulation	The estimated steady-state bioconcentration factor for aquatic organisms containing 7.6% lipids is 11700. Although polycyclic aromatic hydrocarbons are rapidly bioaccumulated, those containing 4 or fewer aromatic rings may also be rapidly metabolized by multicellular organisms. Bioaccumulation is considered to be short-term. – In most cases, PAHs are less bioavailable when complexed to colloidal organic materials or adsorbed to organis or inorganic particulated then when in solution or in fine dispersion in water. For example, the deposit-feeding clam Tacoma inquinata exhibited bioaccumulation factors of 0.04 and 694 when exposed for 7 days to chrysene in contaminated sediments and seawater, respectively. – The long-lived and pollution-tolerant freshwater mollusc Cipangopaludina chinensis (a snail), which is a mucociliary and bottom feeder, showed a bioaccumulation factor of approximately 100 for chrysene in its soft tissues (dry weight basis) compared to the chrysene concentration in the dry sediment from a marsh in a highly populated area. – A bioaccumulation factor of 8.2 was reported for chrysene by the estuarine clam Rangia cuneata when exposed ot 0.066 ppm for 24hr. After 24hr in clean water, 26% of the chrysene had been released. – Pink shrimp Penaeus duorarum was exposed to 0.001 or 0.005 ppm chrysene in seawater. Highest concentrations after 28 days were in the cephalothorax and abdomen. They released most of the chrysene in 10 days after returning to clean seawater, but small amounts still remained after depuration fo 28 days (Sax 1986).
TDLo values to mammals in non-oral exposure, mg/kg	3.6 skn-mus, tumorigenic 200 scu-mus, tumorigenic (Sax 1986)
Health effects	Polycyclic aromatic hydrocarbons can presumably be absorbed from ingestion, inhalation and skin contact. Chrysene is a weak carcinogen (Sax 1986).
Carcinogenicity	In mice, chrysene caused skin tumors after dermal exposure at high concentrations. it was also an initiator in skin carcinogenesis. A low incidence of tumors occurred after scu injection at high doses in mice. – Chrysene is a carcinogenic suspect agent (Sax 1986).

Mutagenicity	Mutagen data: mma, sat, 0.010 mg/plate; msc, hmn, lym, 0.006 mmol/l; msc, mus, orl, 450 mg/kg; otr, ham, kdy, 0.025 mg/l; otr, ham, emb, 5 mg/l; dnd, ham, emb, 1 mg/l; sce, ham, ipr, 900 mg/kg, 24hr (Sax 1986). In the Salmonella test: positive 38 revertant colonies/nmol 1670 revertant colonies at 0,01 mg/plate (Mc Cann et al. 1975)
Effects on invertebrates	Neanthes arenaceodentata, 96hr, LC50, > 1 mg/l (Sax 1986).
Effects on wastewater treatment	Polychlorinated PAHs are probably highly toxic to aquatic organisms and persistent in the environment as are polychlorinated biphenyls and polychlorinated naphthalenes. Chlorination for purification of wastewaters or drinking waters containing high concentrations of PAHs may not be advisable. Activated sludge treatment is unable to oxidize PAHs within normal retention times (Sax 1986).
Other information about water organisms	Daphnia magna; lethal threshold concentration, 1 day, 0.0007 mg/l (Newsted & Giesy 1987).

560 • Cinnamaldehyde

104-55-2

Synonyms	Cinnamic aldehyde 3-Phenylpropenal β-Phenylacrolein Cinnamyl aldehyde	
Molecular weight	132.15	
Specific gravity (water=1)	1.112	at 15/4 °C
Conversion factor, 1 ppm in air=	5.493	mg/m^3 (Verschueren 1983)
Conversion factor, 1 mg/m^3 in air=	0.182	ppm (Verschueren 1983)
Vapour pressure, mmHg	1 40	at 76.1 °C at 152 °C
Melting point, °C	-7.5	
Boiling point, °C	251	
Log octanol/water coefficient, log Pow	1.88	(Verschueren 1983)
LD50 values to birds in oral exposure, mg/kg	> 96.0	orl-Agelaius phoeniceus (Schafer et al. 1983)

561 • Cinnamic acid

621-82-9

Synonyms	3-Phenylpropenoic acid Cinnamylic acid
Sumformula of the chemical	$C_9H_8O_2$
Use	Medicine (anthelmintic), perfumes, intermediate.
State and appearance	White, crystalline scales.

Boiling point, °C	246	(MITI 1992)
pKa	4.2	about 4.2 (Sangster 1989)
Log octanol/water coefficient, log Pow	2.1 2.25	(Anon. 1986) (Sangster 1989)
Other physicochemical properties	Soluble in benzene, ether, acetone, glacial acetic acid, carbon disulfide, oils; insoluble in water.	
Total degradation in water	Biodegradation: 77.2–92.0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

562 • Cinnamic alcohol

104-54-1

Synonyms	Cinnamyl alcohol Phenyl allylic alcohol 3-Phenyl-1-propen-1-ol Styryl carbinol	
Sumformula of the chemical	C9H10O	
Use	Perfumery, particularly for lilac and other floral scents; flavoring agent; soaps; cosmetics.	
State and appearance	White needles or crystals.	
Odour	Hyacinthlike odour.	
Boiling point, °C	257	
Log octanol/water coefficient, log Pow	1.9 1.95	(Anon. 1986) (Sangster 1989)
Other physicochemical properties	Soluble in water, alcohol, glycerol and organic solvents. Combustible.	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	

563 • Ciodrin

7700-17-6

Synonyms	O,O-Dimethyl-O-(1-methyl-2-carboxy-α-phenylethyl)-vinylphosphate Crotoxyphos	
Molecular weight	314.3	
LD50 values to mammals in oral exposure, mg/kg	74 125	orl-rat (Lewis & Sweet 1984) orl-rat (Verschueren 1983)
LD50 values to mammals in non-oral exposure, mg/kg	202 385	skn-rat (Lewis & Sweet 1984) skn-rat (Anon. 1976)
LD50 values to birds in oral exposure, mg/kg	111 56.2	orl-ckn (Lewis & Sweet 1984) orl-Agelaius phoeniceus (Schafer et al. 1983)
LC50 values to crustaceans, mg/l	0.011 0.015	96hr, Gammarus fasciatus (Sanders 1972) 96hr, Gammarus lacustris (Sanders 1969)

LC50 values to fishes, mg/l	0.055 0.25 1.1 2.5	96hr, Salmo gairdneri 96hr, Lepomis macrochirus 96hr, Micropterus salmoides 96hr, Ictalurus punctatus (Verschueren 1983)

564 • Citral

5392-40-5

Sumformula of the chemical	C10H160
Melting point, °C	< -10 (MITI 1992)
Boiling point, °C	226–228 (MITI 1992)
Total degradation in water	Biodegradation: 88–94% by BOD period: 28d substance: 100mg/l sludge: 30 mg/l (MITI 1992).

565 • Citrazinic acid

99-11-6

Synonyms	2,6-Dihydroxyisonicotinic acid
Use	Competing coupler in colour developer solution.
Molecular weight	155.11
Melting point, °C	> 300 °C
Other information about degradation	BOD5/COD = 0.092 (Anon. 1974)
LD50 values to birds in oral exposure, mg/kg	> 104 orl-Agelaius phoeniceus (Schafer et al. 1983)
Effects on wastewater treatment	Impact on conventional biological treatment systems: chemical conc. mg/l — effect unacclimated system 320 — no effect 500 — no effect acclimated system 1,010 — no effect The compound did not affect either the unacclimated or acclimated systems however, ther was no evidence to indicate that the compound was biodegradable under either condition (Anon. 1974).
LC50 values to crustaceans, mg/l	32 48hr, Daphnia magna (Verschueren 1983)
LC50 values to fishes, mg/l	> 100 mg/l, Phimephales promelas (Anon. 1974)
Other information about water organisms	EC 100 mg/l, rpd, schr, Selenastrum capricornutum (Verschueren 1983). Biological effects: Selenastrum capricornutum: 1 mg/l, no effect 10 mg/l, no effect 100 mg/l, inhibitory (Anon. 1974)

566 • Citric acid

77-92-9

Synonyms	2-Hydroxy-1,2,3-propanetricarboxylic acid β-Hydroxytricarballylic acid
Molecular weight	192.12
Specific gravity (water=1)	1.542 at 18/4 °C
Water solubility, mg/l	1330 cold
Melting point, °C	153
Log octanol/water coefficient, log Pow	-1.72 (Verschueren 1983)
Other physicochemical properties	Decomposes.
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): Pseudodomonas putida > 10 000 mg/l (Bringmann & Kühn 1980).
LOEC values to algae, mg/l	80 rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
Other information about water organisms	LC100, 120 mg/l, act, Daphnia magna (Ellis 1937). Toxicity threshold (cell multiplication inhibition test): Microcystis aeruginosa 80 mg/l (Bringmann & Kühn 1976) Scenedesmus quadricauda 640 mg/l (Bringmann & Kühn 1980a) Entosiphon sulcatum 485 mg/l (Bringmann & Kühn 1980a) Uronema parduczi Chatton-Lwoff 622 mg/l (Bringmann & Kühn 1980b) LD0, 80 mg/l, Daphnia magna, long time exposure in solf water. LD100, 120 mg/l, Daphnia magna, long time exposure in soft water. (Verschueren 1983) Carassius auratus: period of survival: 4–48hr: 894 ppm at pH 4.0 days: 625 ppm at pH 4.5 (Verschueren 1983) LD0, 625 mg/l, Carassius auratus, long time exposure in hard water. LD100, 894 mg/l, Carassius auratus, long time exposure in hard water. (Verschueren 1983)

567 • CL 38906

10191-74-9

Other information about mammals	ALD = 2.4 mg/kg, act, orl, deer mouse; LDfr = 25.0 mg/kg, subacute, deer mouse (Virtanen & Nuuja 1987).

568 • CMU

150-68-5

Synonyms	3-(p-Chlorophenyl)-1,1-dimethylurea N'(4-Chlorophenyl)-N,N-dimethylurea Monouron Chlorfenidim Telvar 3-(4-Chlorophenyl)-1,1-dimethylurea
Sumformula of the chemical	C9H11ON2Cl
Use	Herbicide, inhibitor of photosynthesis and is absorbed via the roots, sugarcane flowering supressant.
State and appearance	White, chrystalline solid.
Odour	Odourless.

Specific gravity (water=1)	1.27 at 20/20 °C
Vapour pressure, mmHg	0.0000005 25 °C
Water solubility, mg/l	230 25 °C
Melting point, °C	174
Log soil sorption coefficient, log Kom	1.46 (Sabljic 1987)
Other physicochemical properties	Very low solubility in water and hydrocarbon solvents, slightly soluble in oils, partially soluble in alcohols, stable toward oxidation and moisture.
Half-life in soil, days	166 (Li et al. 1990)
Total degradation in water	persistence in river water in a sealed glass jar under sunlight and artifical fluorescent light -initial conc. 10 E-6 g/l *% of original compound found* after: 1hr 80; 1wk 40; 2wk 30; 4wk 20; 8wk 0 (Eichelberge & Lichtenberge 1971)
Other information about degradation	Aquatic reactions: 75–100% disappearance from soils: 10 months (Verschueren 1983).
LD50 values to mammals in oral exposure, mg/kg	3600 orl-rat (Anon.1976)
Health effects	In diet: rats and dogs: no effect level: 250-500 ppm (Martin 1968).
EC50 values to algae, mg/l	90 pht, schr, Phaeodactylum tricornutum (Walsh 1972)
LOEC values to algae, mg/l	1 rpd, schr, Dunaliella euchlora 1 rpd, schr, Phaeodactylum tricornutum (Ukeles 1962)
Effects on the reproduction of water organisms	Chlorococcum sp. 100ppb: 54% inhibition of growth: 10 day growth test (Walsh & Grow 1971) Dunaliella tertiolecta 150ppb: 50% decrease growth: 10 day growth test (Walsh 1972)

569 • Co-ral * 56-72-4

Synonyms	Muscatox Resistox Coumaphos Bay 21/199 Asuntol Baymix Meldane 0,0-Diethyl-0-(3-chloro-4-methyl-2-oxo(2H)-1-benzopyran-7-yl)-phosphorothioate 3-Chloro-4-methyl-7-courmarinyl diethylphosphorotionate
Active ingredients	3-Chloro-4-methyl-7-cumarinyl-diethylphosphorothioate
Use	Insecticide.
State and appearance	Tan crystalline solid.
Specific gravity (water=1)	1.47 at 20/4°
Vapour pressure, mmHg	0.0000001 at 20 °C
Melting point, °C	90–92 °C
Hydrolysis in base	Hydrolyses slowly under alkaline conditions.

LD50 values to mammals in oral exposure, mg/kg	56–230 41 15.5	mg/kg (techn. grade), orl-rat orl-male-rat (Anon. 1963) orl-female-rat (Martin 1968)
LD50 values to mammals in non-oral exposure, mg/kg	860	n-male-rat (Martin 1968)
Effects on arthropods	LC50, 0.005 mg/l, 24hr, Hydropsyche sp. LC50, 0.43 mg/l, 24hr, Hexagenia sp. (Verschueren 1983)	
LC50 values to crustaceans, mg/l	0.000007 0.001 0.00015	96hr, Gammarus lacustris (Sanders 1969) 48hr, Daphnia magna (Sanders 1972) 96hr, Gammarus fasciatus (Sanders 1972)
LC50 values to fishes, mg/l	18 0.18 1.5 15	96hr, Pimephales promelas 96hr, Lepomis macrochirus 96hr, Salmo gairdneri 96hr, Oncorhynchus kisutch (Katz 1961)

570 • Cobalt and cobalt compounds 7440-48-4

Molecular weight	58.93	
LDLo values to mammals in oral exposure, mg/kg	1500 20	orl-rat orl-rbt (Lewis & Sweet 1984)
Effects on amphibia	LC50 (96hr), 17.59 ppm, tadpoles of Rana hexadactyla (Khangarot et al. 1985).	
Effects on plants	Root tips of horse-bean (Vicia faba L.) seedlings were kept in vessels containing 0.001% solutions of cobalt (Co(NO3)2) for 2 hours -> destructions of the cell division (Herichova 1974). Two cultivars of cotton (Gossypium spp.) were grown in solution culture. Leaf yields of one cultivar were depressed 82% by 0.0001 M CoSO4 (leaf concentration was 0.180 mg Co/g). Plants were tolerant of mg/g of about 0.069 Co (Rehab & Wallace 1978a). Two cultivars of cotton (Gossypium spp.) were grown in Yolo loam soil in pots. Leaf yields were depressed 98% and 92% by 0.400 mg Co/g soil (leaf metal concentration were 0.243 and 0.224 mg Co/g) (Rehab & Wallace 1978b).	
EC50 values to algae, mg/l	0.018 0.016	rpd, 96hr, Selenastrum capricornutum rpd, 7d, S. capricornutum (Chiaudani & Vighi 1978)
LC50 values to crustaceans, mg/l	0.021 1.11 1.62	21d, Daphnia magna 48hr, without food, D.magna 48hr, with food, D.magna (Biesinger & Christensen 1972)
EC50 values to crustaceans, mg/l	0.012	rpd, 21d, Daphnia magna (Biesinger & Christensen 1972)
LOEC values to crustaceans, mg/l	0.01	21d, rpd, Daphnia magna (Biesinger & Christensen 1972)
LC50 values to fishes, mg/l	0.49	28d, Salmo gairdneri (Birge et al. 1980)

571 • Cobalt chloride 7646-79-9

EC50 values to algae, mg/l	23.8 14.4 10.9 8.13	4d, Spirulina platensis 5d, Spirulina platensis 6d, Spirulina platensis 7d, Spirulina platensis (Sharma et al. 1987)
LC50 values to crustaceans, mg/l	2.11 1.52	1d, Daphnia magna 2d, Daphnia magna (Khangarot et al. 1987)
EC50 values to crustaceans, mg/l	167 39.2	2d, mbt, Crangonyx pseudogracilis 4d, mbt, Crangonyx pseudogracilis (Martin & Holdich 1986)

C

572 • Consin 57017-81-9

LC50 values to fishes, mg/l	600	96hr, Rasbora heteromorpha (Tooby et al. 1975)

573 • Copper acetate 142-71-2

LC50 values to crustaceans, mg/l	37	96hr, Palaemonetes pugis (Curtis et al. 1979)
LC50 values to fishes, mg/l	0.39	96hr, Pimephales promelas (Curtis et al. 1979)

574 • Copper and copper compounds 7440-50-8

Sumformula of the chemical	Cu
Molecular weight	63.54
Mobility	Copper is found in soil in many ion forms: mono and bivalent ion forms and cat-ion and anion complexes. Cu2+ seems to be the most mobile ion form. Chelate and complex forming are key reactions in most soil types. Generally copper seems to be one of the least mobile metals in the soil (Walterson 1987). Cu2+ in fresh waters is usually bind to complexes. Only 1% appears generally as free Cu2+. In waters containing little humus, the appearance (Cu2+, OH- and CO3-complexes) is influenced by pH and alkalinity, in sea water also chloride concentration (Spear & Pierce 1979). Cu is calculated to appear in sea water, in pH 7.8 mostly as soluble Cu(OH)2 (80%) and soluble CuCO2-complex (20%) (Zirino & Yamamoto 1972).
Bioconcentration factor, algae	17000 plankton, calc. (Bowen 1966) 360–9300 phytoplankton (Cushing & Rancitelli 1972)
Other information about bioaccumulation	With higher salinity and higher pH the uptake of copper decreases (Bowen 1966). Bioaccumulation is decreased with higher trophic level; so there is no tendency to biomagnification (Spear & Pierce 1979).
TDLo values to mammals in oral exposure, mg/kg	0.12 orl-hmn (Lewis & Sweet 1984)
Teratogenicity	Teratogenic effects of high copper intake with mothers has not been noticed, on the other hand deficiency of copper can induce severe disturbances in development (Nyholm 1985).
Effects on amphibia	LC50 (96hr), 0.039 mg/l, tadpoles of Rana hexadactyla (Khangarot et al. 1985).

Effects on plants	Soybean seeds (Glycine max) were planted in acid-washed sand. Beginning 5 days after seed germination the sand was saturated with metal solutions: Cu at 1 ppm caused reductions in stem and foliage dry weights (leaves and stems contained 0.00287 mg Cu/g) (Vesper & Weidensaul 1978).
EC50 values to algae, mg/l	0.002–0.005Thalassiora pseudonana (Spear & Pierce 1979)
LOEC values to algae, mg/l	0.05 rpd, schr, Selenastrum capricornutum (Bartlett et al. 1973) 0.25 rpd, chr, Chlorella saccorophila (Aliotta & Pollio 1982) 0.01 oligotrophic, Sceletonema costatum 0.5 rich with phosphate, S. costatum (Spear & Pierce 1979)
LC50 values to crustaceans, mg/l	0.026 48hr, Daphnia magna (Lewis 1983) 0.017–0.096 96hr, Gammarus pulex (Stephenson 1983) 0.044 21d, Daphnia magna 0.0098 48hr, without food, D.magna 0.06 48hr, with food, D.magna (Biesinger & Christensen 1972) 0.212 4hr, Gammarus lacustris (DeMarch 1988)
EC50 values to crustaceans, mg/l	0.035 21d, rpd, Daphnia magna (Biesinger & Christensen 1972)
LOEC values to crustaceans, mg/l	0.022 21d, rpd, Daphnia magna (Biesinger & Christensen 1972)
LC50 values to fishes, mg/l	0.017 96hr, Oncorhynchus kisutch (Buckley 1983) 3 24hr, Barbus ticto ticto (Saxena & Parashari 1983) 0.11 28d, Salmo gairdneri (Birge et al. 1980) 0.1 96hr, sfd, Morone saxatilis 0.27 96hr,hrd, Morone saxatilis 0.19 96hr, 1%, Morone saxatilis (Palawski et al. 1985) 0.075 96hr, 30 mg CaCO3/l, Pimephales promelas 0.47 96hr, 198 mg CaCO3/l, P. promelas (Spear & Pierce 1979) 0.032–0.125 96hr, 8–20 mg CaCO3/l Salmo salar 0.017–1.1 96hr, 21–371 mg CaCO3/l Salmo gairdneri (USEPA 1980)
EC50 values to fishes, mg/l	2 48hr, Ictalurus punctatus (Huey et al. 1984)
LOEC values to fishes, mg/l	0.0000007 Salmo gairdneri (Buckley et al. 1984) 0.021 srv, grw, schr, Oncorhynchus tshawytscha (Hazel & Meith 1970) 0.017 srv, grw, Salmo trutta m. lacustris (McKim & Benoit 1971) 0.04 grw, chr, Lepomis macrochirus (Benoit 1975) 0.018 srv, rpd, chr, Pimephales promelas 0.033 rpd, chr, Pimephales promelas (Mount & Stephan 1969) 0.118 rpd, chr, Pimephales promelas (Brungs et al. 1976) 0.018 rpd, chr, Phoxinus phoxinus (Horning & Neihesel 1979) 0.005–0.007 2mo, Salvelinus fontinalis embryo/larvae (McKim et al. 1978)

NOEC values to fishes, mg/l	0.04	srv, grw, Salmo trutta m. lacustris (McKim & Benoit 1971)
	0.021	grw, chr, Lepomis macrochirus (Benoit 1975)
	0.011	srv, rpd, chr, Pimephales promelas
	0.015	rpd, chr, Pimephales promelas (Mount & Stephan 1969)
	0.066	rpd, chr, Pimephales promelas (Brungs et al. 1976)
	0.004	rpd, chr, Phoxinus phoxinus (Horning & Neihesel 1979)
Other information about water organisms	LC50 (96hr) = 0.3 mg/l; LC50 (20d) = 0.08 mg/l, Chironomus tentans (Nebeker et al. 1984).	
	LC50 (96hr), 0.034 mg/l, Lymnea acuminata (Khangarot et al. 1982).	
	Algae, 14d, 0.100 mg/l, biomass effect (Kerrison et al. 1988).	
	Aquatic community, 0.0025–0.015 mg/l, change in number of species groups (Leland et al. 1988).	
	Gambusia affinis, 2d, 0.160 mg/l, mortality (Chagnon & Guttman 1988).	
	Epeorus latifolium (Ephemeroptera), LOEC, 0.010–0.015 mg/l, growth of larvae (Hatakeyama 1989).	
	Daphnia, impaired reproduction ability, 0.022–0.035 (sft), 0.04–0.08 (hrd) (Balsberg et al. 1981).	
	Asellus aquaticus, chronic exposure, 0.005 mg/l, juvenile growth inhibited (Giudici et al. 1988).	
	Acartia calusi (marine copepod), chronic exposure, 0.001–0.01 mg/l, rpd, mortality (Moraitou-Apostolopoulou & Verriopoulus 1979).	
	Mytilus edulis, 0.01–0.02 mg/l, disturbance of early developing stages (Swedmark et al. 1978).	
Other information	Copper is essential in many copper enzymes. Copper metabolism is influenced by many inorganic substances, mostly calcium, cadmium, zinc, iron, lead, molybdene and sulfate (Nyholm 1985).	

575 • Copper(I) chloride 7758-89-6

Sumformula of the chemical	ClCu	
Molecular weight	98.99	
LD50 values to mammals in oral exposure, mg/kg	265	orl-rat (Lewis & Sweet 1984)

576 • Copper(II) chloride 7447-39-4

Sumformula of the chemical	Cl2Cu	
Molecular weight	134.44	
Water solubility, mg/l	1000000	CuCl2 x 2 H20, 25 °C
LD50 values to mammals in oral exposure, mg/kg	140	orl-rat
	190	orl-mus
	31	orl-gpg (Lewis & Sweet 1984)
LDLo values to mammals in non-oral exposure, mg/kg	100	scu-gpg (Lewis & Sweet 1984)
EC50 values to crustaceans, mg/l	0.0161	21d, Daphnia magna (Van Leeuwen et al. 1988)

LC50 values to fishes, mg/l	0.06	96hr, Oncorhynchus kisutch (Lorz & McPerson 1977)
	0.069	21d, Daphnia magna (Van Leeuwen et al. 1988)
Effects on the physiology of water organisms	Daphnia magna, 21d, 0.0126–0.0368 mg/l, growth effect (Van Leeuwen et al. 1988).	
	Lepomis macrochirus, 7d, 0.770 mg/l, physiological effect (Heath 1987).	

577 • Copper(II)hydroxide carbonate 12069-69-1

Synonyms	Basis copper carbonate Basic cupric carbonate Dicopper dihydroxycarbonate Malachite	
Sumformula of the chemical	CH2Cu2O5	
EINECS-number	2351136	
Purity, %	> 98	(WPSREG 1993)
Known impurities	Na 0.3–0.4% Zn 0.01–0.14% Fe 0.007–0.1% Pb < 0.005% Cd < 0.0001% Mg 0.03–0.04% Cl 0.15–0.10% S < 0.02% water 0.4–2.0% Ca 0.1–0.25% insoluble material 0.1–0.05% (WPSREG 1993)	
Use	Active ingredient in liquid wood preservatives with preventive efficancy against wood-destroying fungi including softrot and wood-destroying insects (WPSREG 1993).	
State and appearance	solid	(WPSREG 1993)
Density, kg/m³	3700	(WPSREG 1993)
Water solubility, mg/l	0.8	(WPSREG 1993)
Melting point, °C	200	degrades at 200° C (WPSREG 1993)

578 • Copper nitrate 3251-23-8

Synonyms	Copper(2)nitrate Cupric nitrate Nitric acid, copper (2+) salt Copper dinitrate Copper (II) nitrate
Sumformula of the chemical	Cu. (NO3)2
Use	Textile dyeing; chemicals production; pyrotechnics; electroplating; photocopy photography; insecticides.
State and appearance	Large blue-green deliquescent orthorhombic crystal. Will be dissolved in water.
Odour	Lower taste threshold: 0.001 ppm; upper taste threshold: 12.7 ppm (Sax 1986).
Molecular weight	187.56
Specific gravity (water=1)	2.32

C

Boiling point, °C	170
Sublimation point, °C	255
Other physicochemical properties	1 mg/l of Cu reacts with soap to produce insoluble green curds, and blue-green stain on porcelain fixtures. Accelerates the corrosion of Al and Zn (Sax 1986). Flammability: Slight. Combustion requires preheating (Sax 1986). Toxic combustion products: Slightly hazardous (Sax 1986). Explosiveness: Stable (Sax 1986). Misciple at 25 °C.
Other information about bioaccumulation	Cu is not cumulative systemic poison. Most is excreted. Cu is concentrated by plankton by factors of 1000 x – 5000 x or more. Oysters cultured in sea water containing 0.13–0.50 mg/l of Cu deposited the metal in their bodies and became unfit as a food substance (Sax 1986). Can be concentrated by food chain (Sax 1986).
Other information about mammals	Trace amounts of Cu are necessary in the diet (Sax 1986). 2–4 mg, daily, rats harmless; 6–9 mg daily, rats, harmful; > 1 mg/kg, 5d, rats, injurious to growth; 1 g, daily, dogs, safe; > 1 g, daily, dogs, fatal; 2 g, daily, sheep, died; 25 mg, daily, sheep, toxic; 500 mg/kg, chickens, minimum toxic level; 5 g, daily for 18 months, cattle, can tolerate: 1.5 g CuS04, daily for 30–80 days, sheep, chronic poisoning; 1 mg/CuS04, daily, pigs, therapeutic dose for anemia; 2500 mg/l CuS04 in drinking water, turkeys, harmful (Sax 1986).
Health effects	Cu deficiency in animals is associated with a severe anemia, because Cu is the active agent in the synthesis of hemoglobin (Sax 1986). Direct contact: Skin and mumem irritation. General sensation: Acid solution 60–100 mg taken orally cause symptoms of gastroenteritis, with nausea and intestinal irritation. 10–30 mg/day causes no effects. Probably only doses of > 100 mg are injurious. Acute hazard level: Mild irritant and allergen. Moderately toxic when ingested or inhaled. Chronic hazard level: Chronic Cu poisoning among humans has never been proved. Considered a slight hazard (Sax 1986). Skin and eye irritation data: skn, rbt, 500 mg, severe; eye, rbt, 100 mg, severe; eye, rbt, 100 mg, 4 s, rns, severe (Sax 1986).
Effects on plants	In the presence of 0.01 mg/l Mo, concentrations of 0.0001–0.01 mg/l Cu had marked effect on the growth of tomatoes (Sax 1986). 20 mg/l, oats, stunts growth; 0.17–0.20 mg/l, sugar beets, barley, toxic; 0.02 mg/l, tomatoes, adequate, in nutrient solution; 2 mg/l, tomatoes, toxic, in nutrient solution; 0.1 mg/l, orange and mandarin seedlings, toxic, in nutr. sol.; 0.5 mg/l, flax, very toxic, water culture; 6.4–31.8 mg/l, sugar beets, potatoes, tomatoes, sand culture, injurious; 6.4–31.8, oats and kale, sand culture, not injurious; 425 mg/l, cress and mustard seeds, solution culture, delayed germination and retarded growth; 106 mg/l, cress and mustard seeds, solution culture, retarded growth; 1 mg/l, peas and barley, nutrient solution, stops root growth; 2 mg/l, oats, slight chlorosis; 10 mg/l, oats, severe chlorosis (Sax 1986).

Effects on wastewater treatment	8.4–35 ppm inhibits sewage 50% (Sax 1986).	
LC50 values to fishes, mg/l	0.25	96hr, Salmo gairdneri (Hale 1977)
	0.093	96hr, Gambusia affinis (Joshi & Rege 1980)
	4	96hr, Channa punctata (Mishra & Srivastava 1980)
Effects on the physiology of water organisms	Cu increases susceptibility of salmon and other fish to lethal ulceration from Acromonas liquefaciens. Relation sited to hemachromatosis (Sax 1986). 0.0549–0.100 mg/l, 1–7d, Salmo gairdneri, physiological effect; 0.055 mg/l, 28d, Salmo gairdneri, physiological effect (Lauren & McDonald 1987a & b).	
Other information about water organisms	5 mg/l, 11hr, Salmo gairdneri, death; 5 mg/l, 13hr, Petromyzon marinus, death; 5 mg/l, 24hr, Lepomis macrochirus, no effect; 0.0188 mg/l, tadpoles, death; 0.1–1.0 mg/l, most fish, not toxic; 1.5 mg/l Cu, 48–72hr, Nereis sp.; toxic threshold; 0.5 mg/l Cu, 96hr, Nereis sp.; toxic threshold; 1–2 mg/l Cu, shore crab; toxic threshold; 0.5 mg/l Cu, prawns, toxic threshold; 0.02 mg/l Cu, stickleback, toxic limit; 1 mg/l Cu, Lebistis reticulatus, killed; 0.1 mg/l Cu, Bufo valliceps, killed; 0.1 mg/l Cu, Daphnia magna, killed; 0.4–0.5 mg/l Cu, 48hr, Salmo gairdneri, killed; 0.015–3.0 mg/l, some fish, crustacea, molluscs, insects, phytoplankton, zooplankton; toxic; 0.1–0.5 mg/l, oysters, toxic; 10–30 mg/l, 2hr, barnacles & related species, killed; 0.22–1.0 mg/l, 48–240hr, barnacles & related species, killed; 0.55 mg/l, 12hr, mussel, killed; 0.1–0.5 mg/l, bacteria and microorganisms, toxic; 0.1 mg/l, 48–120hr, giant kelp, photosynthesis is inhibited 50%; 0.1 mg/l, 240hr, giant kelp, visible injury (Sax 1986).	
Other effects on aquatic ecosystems	Copper and Cl together increase the toxicity of each alone to Chironomus larvae. Cu and Hg, and Cu and pentachlorophenate are synergistic. Zn and Cu together are much more toxic than either separately in soft water. The effect is not so obvious in hard water (Sax 1986). Sodium nitrite and sodium nitrate decrease the toxicity of some Cu compounds to fish, and Cu decreases the toxicity of cyanide (Sax 1986).	
Other information	Cu chelated by citrate or lignin is just as effective in controlling algae as the free Cu ion, but is not toxic toward fish (Sax 1986). Causes undesirable colour reactions in food-preserving industries. Causes fatty, oily, fishy tastes in milk products. Traces in metal-plating baths affect the smoothness and brightness of the finish. Accelerates corrosion os Al and Zn especially. Absorbed readily on wool, and causes holes when the wool is bleached. Reclaimed rubber processed with water with 10– 25mg/l Cu deteriorated more rapidly than rubber processed with no Cu present (Sax 1986).	

579 • Copper sulfate

7758-98-7

Sumformula of the chemical	CuSO4
Use	Fungicide.
Molecular weight	159.6

C

Water solubility, mg/l	316000	$CuSO_4 \times 5 H_2O$, 0 °C
LD50 values to mammals in oral exposure, mg/kg	300	orl-rat (Lewis & Sweet 1984)
TDLo values to mammals in oral exposure, mg/kg	11	orl-hmn (Lewis & Sweet 1984)
LDLo values to birds in oral exposure, mg/kg	600	orl-dck (Lewis & Sweet 1984)
Effects on invertebrates	Invertebrates; 0.550 mg/l, 4d, abundance effect (number of organisms in the same species changes) (Hawkins & Griffiths 1987).	
Effects on arthropods	Chironomus decorus: EC50, grw, 15d, 1602 mg/kg (Kosalwat & Knight 1987b); LC50, 2d, 0.739 mg/l (Kosalwat & Knight 1987a); LC50, 3d, 5830 mg/l (Kosalwat & Knight 1987a); 5.071 mg/l, 3d, effect on hatchability (Kosalwat & Knight 1987b)	
Effects on plants	Growth of mycorrhizal sour orange (Citrus aurantium) seedling was depressed by spraying of soil with 112 kg copper (53% in basic copper sulfate)/ha. Horse-bean (Vicia faba) plants were grown in nutrient solution containing 1 mg Cu/l → changes in the structure of meristemic root cells (Kostal 1974). Two cultivars of cotton (Gossypium spp.) were grown in solution culture. Leaf yields were depressed 76% and 91% by 0.0001 M $CuSO_4$ (leaf concentration were 0.110 mg Cu/g (plants were tolerant of about 0.015 mg Cu/g and 0.065 mg Cu/g) (Rehab & Wallace 1978a).	
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 0.03 mg/l (Bringmann & Kühn 1980a)	
EC50 values to algae, mg/l	0.1	pht, 0.17d, Scenedesmus quadricauda (Starodub et al. 1987)
LC50 values to crustaceans, mg/l	0.58 0.1	1d, Daphnia magna 2d, Daphnia magna (Khangarot et al. 1987a)
	0.093	2d, Daphnia magna (Khangarot et al. 1987b)
	0.1	4d, Macrobrachium carcinus (Correa 1987)
EC50 values to crustaceans, mg/l	9.21 2.44 1.29	4d, mbt, Asellus aquaticus 2d, Crangonyx pseudogracilis 4d, Crangonyx pseudogracilis (Martin & Holdich 1986)
	0.536 0.093	1d, Daphnia magna 2d, Daphnia magna (Khangarot & Ray 1987)
	0.670–5.1	2d, Cypris subglobosa (Khangarot & Ray 1987c)

LC50 values to fishes, mg/l	0.1	96hr, Salmo gairdneri (Lewis & Sweet 1984)
	0.2	96hr, Rasbora heteromorpha (Durve et al. 1980)
	0.3	96hr, Carassius auratus (Tsai & McKee 1980)
	2.54	96hr, Anguilla rostrata (Hinton & Eversole 1978)
	0.1 0.15	96hr, Salmo gairdneri 96hr, Branchydanio rerio (Fogels & Sprague 1977)
	< 0.100–8.0	2d, Salmo gairdneri (Shazili & Pascoe 1986)
	1.9–2.7	1d, Barbus arulius (Shivaraj & Patil 1988)
	0.09196	4d, Barbus gonionotus (Jangchudjai et al. 1987)
	3.2	4d, Clarias lazera (El-Domiaty 1987)
	10.49	4d, Heteropheustes fossilis (Rajbanshi & Gupta 1988)
	1.69 0.829	2d, Mystus bleekeri 4d, Mystus bleekeri (Khangarot & Ray 1988)
	0.25	4d, Pimephales promelas (Scudder et al. 1988)
	0.135 1.38 0.838 3.51 0.884	4d, Salmo gairdneri, 13 °C 4d,hrd, Carassius auratus, 18 °C 4d,hrd, Pimephales promelas, 18 °C 4d, Lepomis cyanellus, 18 °C 4d, Lepomis macrochirus, 18 °C (Johnson & Finley 1980)
Effects on the physiology of water organisms	Channa punctatus; 0.4 mg/l, 14d, biochemical effect (change in physiochemical process including glycogen uptake, cholesterol levels and lipid analysis) (Ansari 1987b). Cyprinus carpio; 2.0 mg/l, 1d, change in enzyme activity (Vig et al. 1987). Salmo gairdneri; 664 mg/kg, 168d, histological effect (presence of physical damage to tissues) (Lanno et al. 1987). Barbus arulius, 2.0 mg/l, 1–4d, oxygen consumption effect (Shivaraj & Patil 1988). Clarias batrachus, 1.0 mg/l, 14d, biochemical effect (Jana & Sahana 1988). Clarias lazera, 3.2 mg/l, 4d, hematological effect (El-Domiaty 1987). Heteropneustes fossilis, 8.17 mg/l, 4d, histological effect (Rajbanshi & Gupta 1988). Heteropneustes fossilis, 0.056 mg/l, 14d, physiological effect (Khangarot et al. 1988). Macrobrachium carcinus, 0.010 mg/l, 0.25d, oxygen consumption effect, physiological effect (Correa 1987). Salmo gairneri: 2.0 mg/l, 1d, enzyme effect (Nemcsok & Hughes 1988); 0.006 mM/l, 1d, mortality (Reid & McDonald 1988); 0.0000021 mM, 2d, physiological effect (Dixon et al. 1987).	

Other information about water organisms	Algae; 0.550 mg/l, 4d, change in biomass (Hawkins & Griffiths 1987). Anacystis nidulans: 0.010 mg/l, 0.25d, pht (Azeez & Banerjee 1987). Spirulina platensis: 0.010 mg/l, 0.25d, pht (Azeez & Banerjee 1987). Asellus aquaticus, 0.005 mg/l, 15–30d, mortality, reproductive effect; Asellus aquaticus, 0.500–15.000 mg/l, 3–40.3d, lethal threshold concentration (LT50) (DeNicola Guidici et al. 1987). Daphnia sp., 0.500 mg/l, 1–56d, mortality (Taub et al. 1988). Ephydatia fluviatilis, 0.0000001 M, 10d, growth effect (Francis & Harrison 1988). LC50, 4 d: Etheostoma flabellare, 0.330–0.392 mg/l; Etheostoma nigrum, 0.493–0.602 mg/l (Lydy & Wissing 1988). LC50, Lymnaea luteola: 2d, 0.052 mg/l; 4d, 0.027 mg/l (Khangarot & Ray 1988). LC50, Polypedilum nubifer, 2d, 0.050–4.3 mg/l (Hatakeyama 1988). Lethal threshold concentration (LT50), Proasellus coxalis, 0.500–15.0 mg/l, 2.33–32.75 d (DeNicola Guidici et al. 1987). Scenedesmus acuminatus, 40 g/m³, 0.02d, mortality (Pekkala & Koopman 1987). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 1.1 mg/l protozoa (Entosiphon sulcatum): 0.11 mg/l (Bringmann & Kühn 1980a)
Other effects on aquatic ecosystems	Algae, 0.500 mg/l, 1–56d, change in cell number of algae species (Taub et al. 1988). Anabaena variabilis, 0.00000079 M, 7d, change in cell number of algae species (Kosakowska et al. 1988). Chlorella vulgaris, 0.00000079 M, 7d, change in cell number of algae species (Kosakowska et al. 1988). Scenedesmus quadricauda, 0.050–0.200 mg/l, 15d, change in cell number of algae species (Starodub et al. 1987b).

580 • Corexit 7664 — 12774-30-0

LC50 values to fishes, mg/l	15.8 96hr, Salmo gairdneri 3200 96hr, Pimephales promelas (Kemp et al. 1973)

581 • Coumaphos — 56-72-4

Synonyms	0,0-Diethyl 0-(3-chloro-4-methyl-2-oxy(2H)1-benzopyran-7-yl-phosphorothioate
Sumformula of the chemical	C14H16ClO5PS
Use	Insecticide; nematocide.
State and appearance	Tan crystalline solid. Will sink and will appear as a layer on the bottom.
Odour	Lower odour threshold: 0.02 ppm (Sax 1986).
Molecular weight	362.78
Specific gravity (water=1)	1.474
Vapour pressure, mmHg	0.0000001 20 °C
Melting point, °C	90–92

Other physicochemical properties	Practically insoluble in water. 1.50 ppm at 25 °C (Sax 1986).	
Hydrolysis in base	Hydrolyzes slowly under alkaline conditions (Sax 1986).	
Other information about degradation	Nonpersistant. Most organophosphates are quite readily hydrolyzed, therefore are not persistent in soils and water. Those not readily hydrolyzed might be expected to be taken up by a wide range of aquatic organisms. However, organophosphates are relatively short lived in biological systems. It is not leached but oxidized in soil and retains its anticholinesterase activity (Sax 1986).	
Other information about metabolism	Food chain contamination potential: moderate. Coumaphos is moderately persistent in the food chain (Sax 1986).	
Other information about bioaccumulation	Organophosphates are highly toxic to birds, mammals, and fish, and would kill the organism before it would be taken into the tissues. Even when these chemicals are taken up by fish, they seldom persist for longer than a week (Sax 1986).	
LD50 values to mammals in oral exposure, mg/kg	13	orl-rat (Lewis & Sweet 1984)
	16	orl-rat
	28	orl-mus
	80	orl-rbt
	58	orl-gpg
		(Sax 1986)
LD50 values to mammals in non-oral exposure, mg/kg	500	skn-rbt (Lewis & Sweet 1984)
	860	skn-rat
	7	ipr-rat
	200	ipr-mus
	140	ipr-gpg
		(Sax 1986)
LC50 values to mammals in inhalation exposure, mg/m³	303	ihl-rat (Lewis & Sweet 1984)
Health effects	Acute poisoning from inhalation or skin absorption may cause headaches, dizziness, weakness, anxiety, tremors of the tongue and eyelids, and impairment of visual acuity. Prolonged contact may result in salivation, tearing, abdominal cramps, vomiting, sweating, and muscular fasciculations. Death can occur from respiratory difficulty, cyanosis, and convulsions. Irritates skin and eyes on contact (Sax 1986).	
Carcinogenicity	NCI carcinogenesis bioassay completed: results negative; mus, rat (Lewis & Sweet 1984).	
LD50 values to birds in oral exposure, mg/kg	14	orl-ckn
	3	orl-bwd
		(Lewis & Sweet 1984)
	1.78–3.6	orl-Agelaius phoeniceus
	75.0–316	orl-Sturnus vulgaris
	13.3	orl-Coturnix coturnix
	10	orl-Passer domesticus
	3.16–4.22	orl-Quiscalus quiscula
	5.62	orl-Columba livia
	2.37	orl-Carpodacus mexicanus
	1	orl-Molothrus ater
	3.16	orl-Quelea quelea
		(Schafer et al. 1983)
Effects on wastewater treatment	Ozone water treatment will increase the toxicity of coumaphos due to the replacement of P:S bonds with the more toxic P:O bonds. Amenable to biological treatment at a municipal sewage treatment plant when diluted (Sax 1986).	

LC50 values to crustaceans, mg/l	0.00007	96hr, Gammarus lacustris
	0.001	48hr, Daphnia magna (Sanders 1972)
	1	48hr, Daphnia magna (Sax 1986)
	0.000074	96hr, Gammarus fasciatus, 21 °C (Johnson & Finley 1980)
EC50 values to crustaceans, mg/l	0.0001	48hr, Simocephalus, first instar, 15 °C (Johnson & Finley 1980)
LC50 values to fishes, mg/l	1.5	96hr, Salmo gairdneri
	0.18	96hr, Lepomis macrochirus (Katz 1961)
	0.5	36hr, Micropterus dolomieu (Sax 1986)
	0.862	96hr, Salmo clarki, 12 °C
	0.89	96hr, Salmo gairdneri, 12°
	0.593	96hr, Salvelinus namaycush, 12 °C
	0.84	96hr, Ictalurus punctatus, 18 °C
	1.1	96hr, Micropterus salmoides, 18 °C
	0.34	96hr, Lepomis macrochirus, 18 °C
	0.78	96hr, Stizostedion vitreum, 18 °C (Johnson & Finley 1980)
EC50 values to fishes, mg/l	0.28	48hr, Longnose killifish, 12 °C (Sax 1986)

582 • Creosote

8001-58-9

Chemicals in the product	* Mixture of above all; phenol type compounds	
Use	Impregnant of wood.	
LC50 values to crustaceans, mg/l	0.02	96hr, Homarus americanus (McLeese & Metcalfe 1979)
	1.76	96hr, 10 °C, Homarus americanus, adult
	0.02	96hr, 20 °C, Homarus americanus, larval
	0.13	96hr, 10 °C, Crangon
	0.11	96hr, 20 °C, Crangon (Verschueren 1983)
Other information	A mixture of phenols and phenol derivatives obtained by the destructive distillation of wood-tar. One of the avtive constituents is creosol (2-methoxy-4-methylphenol) (from beechwood-tar) Also obtained by fractional distillation of coal-tar; contains substantial amounts of naphthalene and anthracene (Verschueren 1983).	

583 • Cresol

1319-77-3

Sumformula of the chemical	C7H8O	
Boiling point, °C	202	(MITI 1992)
Total degradation in water	Biodegradation: 49.7% by BOD (on the upward trend) period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

584 • m-Cresol

108-39-4

Synonyms	3-Hydroxytoluene 3-Methylphenol 3-Cresol
Sumformula of the chemical	C7H8O
State and appearance	Yellowish liquid.
Odour	Odour threshold (tentative): average: 0.2 mg/l range: 0.016–4.0 mg/l Taste threshold conc.: 0.002 mg/l (Verschueren 1983)
Molecular weight	108.15
Specific gravity (water=1)	1.038 at 20/4 °C
Conversion factor, 1 ppm in air=	4.5 mg/m³ (Verschueren 1983)
Conversion factor, 1 mg/m³ in air=	0.22 ppm (Verschueren 1983)
Vapour pressure, mmHg	0.04 20 °C 0.12 30 °C 5 76 °C
Water solubility, mg/l	23500 20 °C 58000 100 °C
Melting point, °C	12
Boiling point, °C	202
Log octanol/water coefficient, log Pow	1.96 1.96/2.01 2.01 (Verschueren 1983) 1.98 (Sangster 1989)
Henry's law constant, Pa x m³/mol	0.07184 calc. (Yaws et al. 1991)
Total degradation in soil	Decomposition period by a soil microflora: 1 day (Verschueren 1983).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
Other information about degradation	Degradation of m-cresol: (see table below)

ENVIRON.	*INIT. mg/l*	*REDOX-COND.*	*TEMP. °C*	*DEGRAD. %/day*	*REF.*
sludge	appr. 50	anaerob.	35	92/28	a
sludge	appr. 50	anaerob.	35	90/35	a
soil suspension	10	aerobic	25	100/1	b

a) Horowitz et al. 1982
b) Alexander & Lustigman 1966
(Anon. 1987b).

75% inhibition of nitrification process in non adapted activated sludge at 11,4 mg/l. (Meinck et al. 1970)

Inhibition of degradation of glucose by Pseudomonas fluorescens at : 40 mg/l.
Inhibition of degradation of glucose by E. coli at: 600 mg/l.
(Bringmann & Kühn 1960)

Decomposition period by a soil microflora: 1 day. (Verschueren 1983)

LD50 values to mammals in oral exposure, mg/kg	242 828 2020 1100	orl-rat orl-mus (Lewis & Sweet 1984) orl-rat orl-rbt (Patty 1967)
LD50 values to mammals in non-oral exposure, mg/kg	620	skn-rat (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	> 113	orl-Agelaius phoeniceus (Schafer et al. 1983)
Maximum longterm immission concentration in air for plants,mg/m³	0.2	VDI 2306
Maximum longterm immission concentration in air for plants,ppm	0.05	VDI 2306
Effects on microorganisms	LD0, 600 mg/l, E. coli (Verschueren 1983) Toxicity threshold (cell multiplication inhibition test): Pseudomonas putida: 53 mg/l (Bringmann & Kühn 1980a)	
EC50 values to microorganisms	515	OECD 209 (Klecka et al. 1985)
LOEC values to algae, mg/l	13 15	rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976) rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
LC50 values to fishes, mg/l	8.9 7 13.6 23 15.9 17–19	96hr, Salmo gairdneri (DeGraeve et al. 1980) egg, 24hr, Salmo trutta (Anon. 1973a) 96hr, Lepomis macrochirus 96hr, Rutilus rutilus (Jones 1971) 96hr, Branchydanio rerio 48hr, Leuciscus idus (Wellens 1982)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): Microcystis aeruginosa 13 mg/l (Bringmann & Kühn 1976) Scenedesmus quadricauda 15 mg/l (Bringmann & Kühn 1980a) Entosiphon sulcatum 31 mg/l (Bringmann & Kühn 1980a) Uronema parduczi Chatton-Lwoff 62 mg/l (Bringmann & Kühn 1980b)	
Other information	Reduction of amenities: approx. conc. causing taste in trout and carp: 10 mg/l. approx. conc. causing taste in fish: 0.2 mg/l (Jones 1971)	

585 • o-Cresol 95-48-7

Synonyms	2-Hydroxytoluene 2-Methylphenol o-Methylphenol o-Cresylic acid o-Toluol 1-Hydroxy-2-methylbenzene 2-Cresol
Sumformula of the chemical	C7H8O

Purity, %	80–98% pure,	
Known impurities	phenol * 2–20%	
Use	Disinfectant; food antioxidant, perfume manufacturing; dye manufacturing; plastics and resins manufacturing. Tricresylphosphate mfg; ore flotation, textile scouring agent, organic intermediate; mfg of salicylaldehyde, coumarin; surfactant; cresylic acid constituent.	
State and appearance	Clear to yellow solid. Liquid in warm temperature. Will sink and dissolve at moderate rate.	
Odour	Phenolic, tarry odour. Recognition odour in air: 0.26 ppm; lower odour threshold; 0.016 ppm; upper odour threshold: 4.1 ppm; medium taste threshold: 0.001 ppm (Sax 1986). Odour threshold: detection: 1.4 mg/l Taste threshold conc.: 0.003 mg/l (Verschueren 1983)	
Molecular weight	108.15	
Specific gravity (water=1)	1.048 1.041	
Vapour density (air=1)	3.72	
Conversion factor, 1 ppm in air=	4.5	mg/m^3 (Verschueren 1983)
Conversion factor, 1 mg/m^3 in air=	0.22	ppm (Verschueren 1983)
Vapour pressure, mmHg	0.24 5	25 °C 64 °C
Water solubility, mg/l	31000 31 56000	40 °C 25 °C 100 °C
Melting point, °C	31	
Boiling point, °C	191	
Flashing point, °C	81	
Log octanol/water coefficient, log Pow	1.98	(Sangster 1989)
Henry's law constant, Pa x m^3/mol	0.08521	calc. (Yaws et al. 1991)
Other physicochemical properties	Flammability: moderate. Combustion with moderate heating. Toxic combustion products hazardous. Explosiveness: Stable. Vapours form explosive mixtures with air.	
Photochemical degradation in water	Photo-oxidation: an aqueous solution of cresol (n.s.i.) is destroyed by photooxidation using visible light as a direct energy source and methyleneblue as a dye-sensitizer. (Sargent & Sanks 1974)	
Total degradation in soil	Decomposition period by a soil microflora: 1 day (Verschueren 1983).	
Ready biodegradability	Confirmed to biodegradable (Anon. 1987).	

C

Other information about degradation

Degradation of o-cresol:

ENVIRONMENT	*INIT.CONC. mg/l*	*REDOX-COND.*	*TEMP. °C*	*DEGRADATION %/day*	*REF.*
water	20	aerobic	25	99/7	a
sludge	appr. 50	anaerobic	35	0/56	b
sludge	appr. 50	anaerobic	35	0/56	b
soil suspension	10	aerobic	25	100/1	c

a) Bunch & Chamber 1967 b) Horowitz et al. 1982
c) Alexander & Lustigman 1966 (Anon. 1987b).

Biodegrades at moderate rate but can alter aesthetics at very low concentration levels (Sax 1986).

Inhibition of nitrification in activated sludge at: 11-16 mg/l (75% reduction) (n.s.i.) (Verschueren 1983)
Inhibition of degradation of glucose by Pseudomonas fluorescens at 50 mg/l.
Inhibition of degradation of glucose by E. coli at: 600 mg/l.
(Bringmann & Kühn 1960)

Decomposition period by a soil microflora: 1 day. (Verschueren 1983)

Other information about bioaccumulation

Potential for accumulation positive. Chronic toxicant properties via all routes suggest accumulative effects (Sax 1986).

LD50 values to mammals in oral exposure, mg/kg

121 orl-rat
344 orl-mus
(Lewis & Sweet 1984)

1350 orl-rat (Sax 1986)

800 orl-rbt (Patty 1967)

LD50 values to mammals in non-oral exposure, mg/kg

890 skn-rbt
1100 skn-rat
(Lewis & Sweet 1984)

1782 skn-rbt, mixed cresols (Sax 1986)

LDLo values to mammals in oral exposure, mg/kg

940 orl-rbt (Sax 1986)

LDLo values to mammals in non-oral exposure, mg/kg

80 ivn-dog
65 scu-rat
410 scu-mus
55 scu-cat
450 scu-rbt
180 ivn-rbt
360 ipr-gpg
(Sax 1986)

TDLo values to mammals in non-oral exposure, mg/kg

4800 skn-mus, 12W-I, tumorigenic (Sax 1986)

Health effects

Jaundice, dermatitis (Sax 1986).

Direct contact: Dangerous to skin and eyes (Sax 1986).

General sensation: Corrosive to body tissues; toxic by inhalation, skin absorption, ingestion. May cause skin eruptions. Absorption may lead to liver and kidney damage (Sax 1986).

Acute hazard level: 8 g can be fatal to a man. Toxic via all routes. Extremely corrosive irritant and allergen. Emits highly toxic vapours when heated to decomposition. Chronic hazard level: Dermatitis and/or liver and kidney damage (Sax 1986).

Skin and eye irritation data:
skn, rbt, 524 mg, 24hr, severe;
eye, rbt, 105 mg, severe (Sax 1986).

Effects on amphibia	LC50, 40 mg/l, 48hr, Mexican axolotl (3-4 w after hatching). LC50, 38 mg/l, 48hr, claved toad (3-4 w after hatching) (Slooff & Baerselmann 1980)	
Maximum longterm immission concentration in air for plants,mg/m³	0.2	VDI 2306
Maximum longterm immission concentration in air for plants,ppm	0.05	VDI 2306
Effects on microorganisms	LD0, 60 mg/l, E. coli (Verschueren 1983) Toxicity threshold (cell multiplication inhibition test): Pseudomonas putida: 33 mg/l (Bringmann & Kühn 1980a)	
Effects on wastewater treatment	940 ppm inhibited 50% sewage organisms subject to chlorination and subsequently lower taste thresholds (Sax 1986).	
LOEC values to algae, mg/l	6.8	rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
NOEC values to algae, mg/l	65	rpd, schr, Selenastrum capricornutum (Slooff et al. 1983)
LC50 values to crustaceans, mg/l	16 16 9.6	48hr, Daphnia magna 48hr, Daphnia cucullata 48hr, Daphnia pulex (Canton & Adema 1978)
	10–100	48hr, shrimp (Sax 1986)
	23 21	48hr, Asellus aquaticus (Slooff 1983) 48hr, Gammarus pulex (Slooff 1983)
LC50 values to fishes, mg/l	18.2 7.9	96hr, Pimephales promelas 96hr, Salmo gairdneri (DeGraeve et al. 1980)
	2	24hr, Salmo trutta (Anon. 1973a)
	13.4	96hr, Pimephales promelas (Pickering & Henderson 1966)
	18 16	96hr, Poecilia reticulata 96hr, Rutilus rutilus (Jones 1971)
	24 10	96hr, Branchydanio rerio 48hr, Leuciscus idus (Wellens 1982)
	13	48hr, Salmo gairdneri (Slooff et al. 1983)
	23.5	Tilapia mossambica (Devi & Sastry 1987)
	10–33	48hr, plaice (Sax 1986)

Other information about water organisms	6–40 mg/l, inhibitory, Scenedesmus; 5–10 mg/l, inhibitory, Macrocystis pyrifera; 55 mg/l, 1hr, killed, sunfish; 60 mg/l, killed, minnow; 70 mg/l, 3hr, killed, roach; 110 mg/l, 5hr, killed, roach; 10 mg/l, 1hr, lethal, perch (Sax 1986). Toxicity threshold (cell multiplication inhibition test): Microcystis aeruginosa 6.8 mg/l (Bringmann & Kühn 1976) Scenedesmus quadricauda 11 mg/l (Bringmann & Kühn 1980a) Entosiphon sulcatum 17 mg/l (Bringmann & Kühn 1980a) Uronema parduczi Chatton-Lwoff 31 mg/l (Bringmann & Kühn 1980b) LC50, 48hr, 165 mg/l, Tubificidae LC50, 48hr, 34 mg/l, Chironomus gr. thummi LC50, 48hr, 135 mg/l, Erpobdella octoculata LC50, 48hr, 160 mg/l, Lymnaea stagnalis LC50, 48hr, 24 mg/l, Dugesia cf. lugubris LC50, 48hr, 75 mg/l, Hydra oligactis LC50, 48hr, 80 mg/l, Corixa punctata LC50, 48hr, 46 mg/l, Ischura elegans LC50, 48hr, 10 mg/l, Nemoura cinerea LC50, 48hr, 50 mg/l, Cloeon dipterum (Slooff 1983)
Other information	Air pollution: high (Sax 1986). Manifacturing source: coal tar refing; petroleum refing; organic chemical mfg.; wood processing. Natural sources (water and air): coal, petroleum, constituent in wood, constituent in natural runoff. Man caused sources (water and air): automobile exhaust, roadway runoff, runoff from asphalt, general use of plastics, petroleum distillates, fuels, perfumes, oils lubricants, metal cleaning and scouring compounds, laboratory chemical, constituent of domestic sewage. (EPA 1975)

586 • p-Cresol 106-44-5

Synonyms	4-Hydroxytoluene 4-Hydroxyphenol 4-Methylphenol	
Sumformula of the chemical	C7H8O	
Use	Intermediate; disinfectant.	
State and appearance	Yellowish liquid.	
Odour	Quality: tarlike hedonic tone: pungent Taste threshold conc.: 0.002 mg/l Odour threshold: detection: 0.2 mg/l (Verschueren 1983)	
Molecular weight	108.15	
Specific gravity (water=1)	1.0347	at 20/4 °C
Conversion factor, 1 ppm in air=	4.5	mg/m³ (Verschueren 1983)
Conversion factor, 1 mg/m³ in air=	0.22	ppm (Verschueren 1983)

Vapour pressure, mmHg	0.04 20 °C 0.11 25 °C 1 53 °C
Water solubility, mg/l	24000 40 °C 53000 100 °C
Melting point, °C	34.8
Boiling point, °C	202
Log octanol/water coefficient, log Pow	1.94 (Anon. 1986) 2.2 (Anon. 1986) 1.92/1.94 (Verschueren 1983) 1.97 (Sangster 1989)
Henry's law constant, Pa x m³/mol	0.86 (Anon. 1988) 0.03971 calc. (Yaws et al. 1991)
Mobility	Equilibrium distribution: *mass %* air 22.58 water 75.58 solid 1.84 (Anon. 1988).
Total degradation in soil	Decomposition period by a soil microflora: 1 day (Verschueren 1983).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
Other information about degradation	Degradation of p-cresol: (see table below)

ENVIRON.	*INIT. mg/l*	*REDOX-COND.*	*TEMP. °C*	*DEGRAD. %/day*	*REF.*
water	1–3	aerobic	20	100/8	a
water	1–3	anaerob.	20	100/41	a
water	100	aerobic	22	70/2	b
water	100	aerobic	22	100/2	b
sediment	100	aerobic	22	100/2	b
sediment	100	aerobic	22	100/4	b
groundwater	~0.2	sulfate reducing	20	90/10	c
sludge	~50	anaerob.	35	51/28	d
sludge	~50	anaerob.	35	100/21	d
soil suspension	10	aerobic	25	100/1	e

a) Delfino & Miles 1985 b) Van Veld & Spain 1983
c) Smolenski & Suflita 1987 d) Horowitz et al. 1982
e) Alexander & Lustigman 1966 (Anon. 1987b).

75% reduction of the nitrification process in non adapted activated sludge at: 16.5 mg/l. (Meinck et al. 1970).
Inhibition of degradation of glucose by Pseudomonas fluorescens at: 30 mg/l.
Inhibition of degradation of glucose by E. coli at: > 1000 mg/l (Bringmann & Kühn 1960).

Biodegradation: decomposition period by a soil microflora: 1 day. (Verschueren 1983)

LD50 values to mammals in oral exposure, mg/kg	207 orl-rat (Lewis & Sweet 1984) 1800 orl-rat (Patty 1967) 1100 orl-rbt (Patty 1967)
LD50 values to mammals in non-oral exposure, mg/kg	160 unk-mus 301 skn-rbt 750 skn-rat (Lewis & Sweet 1984)

LD50 values to birds in oral exposure, mg/kg	> 96.0	orl-Agelaius phoeniceus (Schafer et al. 1983)
Maximum longterm immission concentration in air for plants,mg/m³	0.2	VDI 2306
Maximum longterm immission concentration in air for plants,ppm	0.05	VDI 2306
NOEC values to algae, mg/l	6	Scenedesmus (Meinck et al. 1970)
NOEC values to crustaceans, mg/l	12 6	srv, act, Daphnia rpd, schr, Scenedesmus (Meinck et al. 1970)
LC50 values to fishes, mg/l	7.9	96hr, Salmo gairdneri (DeGraeve et al. 1980)
	4	24hr, Salmo trutta (Anon. 1973a)
	17	24hr, Rutilus rutilus (Jones 1971)
	19	96hr, Pimephales promelas (Vincent et al. 1976)
	7.5	96hr, Salmo gairdneri (Hodson et al. 1984)
	21 17 16	24hr, Carassius carassius 24hr, Rutilus rutilus 24hr, Tinca tinca (Anon. 1973a)
	5	Salmo gairdneri (Verschueren 1983)
Other information about water organisms	EC50 (24hr), 160 mg/l, rpd, Tetrahymena pyriformis (Yoshioka et al. 1985). EC50 (2 d), 168.25 mg/l, grw, Tetrahymena pyriformis (Schultz 1987).	

587 • Crotonaldehyde

123-73-9
4170-30-3

Synonyms	2-Butenal (CAS 4170-30-3) Butenal-2 2-Butenal (E) (CAS 123-73-9) 2-Butenal (trans) (CAS 123-73-9) Crotonic aldehyde
Sumformula of the chemical	C4H6O
Purity, %	93
Use	Manufacture of N-butanol; crotonic acid; sorbic acid.
State and appearance	Colourless liquid. Will dissolve.
Odour	Pungent suffocating odour. Recognition odour in air 21 mg/m³ (Sax 1986). Threshold Odour Concentration (T. O. C.): 0.6 mg/m³ = 0.2 ppm (Verschueren 1983) 0.1 mg/m³ = 0.035 ppm (Stockham et al. 1969) 0.18–0.57 mg/m³ (Verschueren 1983) 0.420 mg/m³ (Verschueren 1983) Reduction of amenities: faint odour: 0.021 mg/l (Verschueren 1983).
Molecular weight	70
Specific gravity (water=1)	0.853
Vapour density (air=1)	2.41

Conversion factor, 1 ppm in air=	2.8	mg/m³ (Verschueren 1983)
Conversion factor, 1 mg/m³ in air=	0.349	ppm (Verschueren 1983)
Vapour pressure, mmHg	19	at 20 °C
Water solubility, mg/l	180000 155000	
Melting point, °C	-60 -75	
Boiling point, °C	102 99 104	 99/104 °C (Verschueren 1983)
Flashing point, °C	13	
Other physicochemical properties	Reactive at high temperature or pressure. May polymerize with acids or bases.	
Other information about degradation	Biodegrades at slow to moderate rate. Bacteria may acclimate and enhance reduction rate (Sax 1986).	
LD50 values to mammals in oral exposure, mg/kg	300 240 160–300	orl-rat orl-mus (Sax 1986) orl-rat (Patty 1967)
LD50 values to mammals in non-oral exposure, mg/kg	25 140 160 160 380 30	14d, skn-gpg scu-rat ipr-mus scu-mus skn-rbt skn-gpg (Sax 1986)
LC50 values to mammals in inhalation exposure, mg/m³	4000 1400	ihl-rat, 30 min (Sax 1986) ihl-rat, 30 min (Verschueren 1983)
LC50 values to mammals in inhalation exposure, ppm	1400	30 min, ihl-rat (Sax 1986)
LDLo values to mammals in non-oral exposure, mg/kg	100 1700	scu-dog scu-gpg (Sax 1986)
TCLo values to mammals in inhalation exposure, mg/kg	12	ihl-hmn, 10 min (Sax 1986)
Health effects	Direct contact causes tearing-acute local irritant; strong lacrimator, vapours extremely damaging to eyes; highly toxic via ingestion or inhalation; ectremely corrosive to skin and eyes; allergen; chronic allergen; chronic toxic effects unknown (Sax 1986). Skin and eye irritation data: eye, hmn, 45 ppm; skn, rbt, 500 mg, open, mild (Sax 1986).	
Mutagenicity	Mutagen data: mmo, sat, 0.100 ml/l; mma, sat, 0.100 ml/l; spm, mus, ipr, 30 mg/kg (Sax 1986).	
Effects on wastewater treatment	200 mg/l is substrate limiting and 50–100 mg/l is nonsubstrate limiting to anaerobic processes (Sax 1986).	

LC50 values to fishes, mg/l	3.5 96hr, Lepomis macrochirus 1.3 96hr, Menidia audens 1.3 96hr, Medinia beryllina (Dawson et al. 1977)
Other information	Air pollution high (Sax 1986).

588 • Cryolite 15096-52-3

Synonyms	Sodium aluminium fluoride
Sumformula of the chemical	Na3AlF6
Use	Raw material in aluminium manufacturing. Insecticide.
LD50 values to mammals in non-oral exposure, mg/kg	1500–2500 24hr, small rodents (Hodge & Smith 1965)
LD50 values to birds in oral exposure, mg/kg	> 100 orl-Agelaius phoeniceus > 100 orl-Sturnus vulgaris (Schafer et al. 1983)
LC50 values to crustaceans, mg/l	5 48hr, Daphnia pulex (Sanders & Cope 1966)
EC50 values to crustaceans, mg/l	5 Daphnia (Sanders & Cope 1966) 10 48hr, Daphnia pulex, first instar, 15 °C 5 48hr, Simocephalus, first instar, 15 °C (Johnson & Finley 1980)
LC50 values to fishes, mg/l	47 96hr, Salmo gairdneri, 12 °C > 400 96hr, Lepomis macrochirus, 24 °C (Johnson & Finley 1986)

589 • o-Cumenyl methylcarbamate 2631-40-5

Sumformula of the chemical	C11H15O2N
Water solubility, mg/l	400 (MITI 1992)
Melting point, °C	89–91 (MITI 1992)
Boiling point, °C	128–129/20 mmHg (MITI 1992)
Log octanol/water coefficient, log Pow	2.27 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	1.9–3.2 6w, Cyprinus carpio, conc 0.3 mg/l < 2.5–15 6w, Cyprinus carpio, conc 0.03 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	16 48hr, Oryzias latipes (MITI 1992)

590 • Cutrin

66555-33-7

Active ingredients	Copper–triethanolamine complexes	
Use	Algicide.	
LC50 values to crustaceans, mg/l	9.9 12.6 11.4 10.2	48hr, Cladocera 48hr, Calanoida 48hr, Cyclopoida 48hr, Ostracoda (Naqvi et al.1985)
LC50 values to fishes, mg/l	0.21 6.4	96hr, Pimephales promelas 96hr, Micropterus salmoides (Skea & Simonin 1979)
	0.24	96hr, Rasbora heteromorpha (Tooby et al. 1975)
	0.17	96hr, Gambusia affinis (Leung et al. 1983)

591 • Cyanatryn

21689-84-9

Use	Herbicide.	
LC50 values to fishes, mg/l	58	96hr, Ctenopharygodon idella (Tooby et al. 1980)

592 • Cyanazine

21725-46-2

Synonyms	Bladex 2-((4-Chloro-6-(ethylamino)-s-triazin-2-yl)amino)-2-methyl-propionitrile 2-Chloro-4-(1-cyano-1-methylethylamino)-6-ethylamino-1,3,5-triazine	
Sumformula of the chemical	C9H13ClN6	
Products containing the chemical	Bladex 500 S C	
Use	Herbicide.	
Molecular weight	240.73	
Log soil sorption coefficient, log Kom	2.3	(Sabljic 1987)
Half-life in soil, days	14	(Li et al. 1990)
LD50 values to mammals in oral exposure, mg/kg	149 141	orl-rat orl-rbt (Lewis & Sweet 1984)
	380	orl-mus (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	1200	skn-rat (Lewis & Sweet 1984)
TDLo values to mammals in oral exposure, mg/kg	250	orl-rat, 6-15d preg. specific developmental abnormalities (Sweet 1987)
Mutagenicity	dlt, dmg, parenteral, 0.332 mmol/l; dlt, dmg, orl, 100 ppm; mma, sat, 5.17 mg/l (Sweet 1987).	
LD50 values to birds in oral exposure, mg/kg	750	orl-dck (Lewis & Sweet 1984)

C

Effects on plants	Soil was amended to give 2.0 ppm by weight of soil of cyanazine–atrazine – susceptible lamb's -quarters (Chenopodium album L.) were killed soon after germination and emergence. Jensen et al. 1977 Cyanazine when applied with a sprayer at 2.24 kg/ha (preemergence or postemergence) killed lamb's-quarters (Chenopodium album) completely. Bandeen & McLaren 1976	
LC50 values to crustaceans, mg/l	15.4	96hr, Daphnia longispina (Verschueren 1983)
LC50 values to fishes, mg/l	4.9	96hr, Salmo trutta (Nikunen et al. 1986)
	15	96hr, Rasbora heteromorpha (Tooby et al. 1975)
	11.3	96hr, Sarotheredon aureus (Rao & Dad 1979)
	18	48hr, Cyprinodon variegatus (Pesticide Manual 1983)
	24.5 12.6	96hr, Sarotherodon mossambicus 96hr, Cirrhinus mrigala (Rao & Dad 1979)

593 • Cyanide 57-12-5

Molecular weight	26.02	
LD50 values to mammals in non-oral exposure, mg/kg	3	ipr-mus (Lewis & Sweet 1984)
EC50 values to microorganism, mg/l	0.02	6hr growth P. putida (Slabbert et al. 1986)
EC50 values to crustaceans, mg/l	1.8	rpd, 48hr, Daphnia (Eckenfelder 1966)
LC50 values to fishes, mg/l	0.028 0.042 0.068	96hr, Salmo gairdneri juv., t= 6 °C 96hr, Salmo gairdneri juv., t= 12 °C 96hr, Salmo gairdneri juv., t= 18 °C (Kovacs & Leduc 1982)
	0.101	96hr, Micropterus salmoides (Smith et al. 1979)
	0.18	24hr, Lepomis humilis (Eckenfelder 1966)
	0.057 0.076 0.053	96hr, Salmo gairdneri 96hr, Perca flavescens 96hr, Salvelinus alpinus (Smith et al. 1978)
LOEC values to fishes, mg/l	0.005	rpd, schr, Lepomis macrochirus (Kimball et al. 1978)
	0.01	srv, grw, schr, Salmo salar (LeDuc 1978)

594 • Cyanogen chloride 506-77-4

State and appearance	Colourless liquid or gas.
Odour	Chracteristic: quality: bitter almonds hedonic tone: pungent Threshold Odour Concentration: 2.5 mg/m³ = 1 ppm (Leonardos et al. 1969). In water: reduction of amenities: faint odour: 0.0025 mg/l (Verschueren 1983).

Molecular weight	61.48	
Specific gravity (water=1)	1.218	at 4/4 °C (Verschueren 1983)
Conversion factor, 1 ppm in air=	2.51	mg/m³ (Leonardos et al. 1969)
Conversion factor, 1 mg/m³ in air=	0.398	ppm (Verschueren 1983)
Vapour pressure, mmHg	1000	at 20 °C (Verschueren 1983)
Water solubility, mg/l	30000	(Verschueren 1983)
Melting point, °C	-6.5	
Boiling point, °C	12.5–13 °C (Verschueren 1983)	
Log octanol/water coefficient, log Pow	0.64	calc (Verschueren 1983)
Other information about mammals	Mouse: inhalation: some deaths: 120 ppm, 3–5 min rabbit: inhallation: fatal: 1200 ppm, 2 min cat: inhalation: fatal: 120 ppm, 3–5 min dog: inhalation: recovered: 20 ppm, 20 min fatal: 48 ppm, 6hr severe injury: 120 ppm 8 min goat: inhalation: fatal after 70hr: 1000 ppm, 3 min (Patty 1967)	
Health effects	Man: fatal after 10 min: 159 ppm 30 min: 48 ppm tolerable for 1 min: 20 ppm 10 min: 2 ppm lowest irritant conc. for 10 min: 1 ppm (Patty 1967).	

595 • 1-Cyanoguanidine 461-58-5

Water solubility, mg/l	41300	(MITI 1992)
Melting point, °C	209	(MITI 1992)
Total degradation in water	Biodegradation: 2.2% by BOD period: 14d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.3 < 3.1	6w, Cyprinus carpio, conc 2 mg/l 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	> 1000	48hr, Oryzias latipes (MITI 1992)

596 • Cyanophos 2636-26-2

Other information about mammals	LDfr = 50.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).	
LC50 values to fishes, mg/l	14	40% product, 48hr, Rasbora heteromorpha (Tooby et al. 1975)

597 • Cyanopyridine 100-48-1

Other information about water organisms	EC50 (60hr) 830 mg/l, rpd, Tetrahymena pyriformis (Schultz & Mouton 1985).

C

598 • Cycloate 1134-23-2

Synonyms	S-Ethyl–N-ethylthiocyclohexanecarbamate Ro-neet	
Use	Active ingredient in herbicides.	
Log soil sorption coefficient, log Kom	2.54	(Sabljic 1987)
LD50 values to birds in oral exposure, mg/kg	> 100 > 100	orl-Agelaius phoeniceus orl-Sturnus vulgaris (Schafer et al. 1983)
Effects on plants	A significant reduction in fresh weight was observed in both sugarbeet cultivars Beta vulgaris Mono Hy A1 and Beta vulgaris Mono Hy D2 and Beta patellaris seedlings growing in soil amended with 4 µg/g cycloate compared with plants growing in nonamended soil (Abivardi & Altman 1978).	
LC50 values to fish	5	96hr, Salmo gairdneri (Anon. 1970)

599 • Cyclododecane 294-62-2

Water solubility, mg/l	< 1	(MITI 1992)
Melting point, °C	63	(MITI 1992)
Boiling point, °C	118	18 mmHg (MITI 1992)
Log octanol/water coefficient, log Pow	> 6.19	(MITI 1992)
Total degradation in water	Biodegradation: 0–12% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	600–3100 1490–7920	10w, Cyprinus carpio, conc 0.03 mg/l 10w, Cyprinus carpio, conc 0.003 mg/l (MITI 1992) (Test I, lipid 3.3%)
	3860–17900 3690–18100	10w, Cyprinus carpio, conc 0.03 mg/l 10w, Cyprinus carpio, conc 0.003 mg/l (MITI 1992) (Test II, lipid 5.4%)
Other information about bioaccumulation	Confirmed to be accumulated on a medium level (Anon. 1987).	
LC50 values to fishes, mg/l	21.8	48hr, Oryzias latipes (MITI 1992)

600 • 1,5,9-Cyclododecatriene 4904-61-4

Synonyms	CDT
Sumformula of the chemical	C12H18
Molecular weight	162.28
Specific gravity (water=1)	0.8925 20/20 °C (Verschueren 1983)
Water solubility, mg/l	< 10 (MITI 1992)
Melting point, °C	-15
Boiling point, °C	231
Log octanol/water coefficient, log Pow	5.5 (Sangster 1989) > 6.19 (MITI 1992)
Chemical oxygen demand, g 02/g	3.02 5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.02 5 days (Bridie et al. 1979)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	2630–12500 10w, Cyprinus carpio, conc 0.01 mg/l 1920–14800 10w, Cyprinus carpio, conc 0.001 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be accumulated on a medium level (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	2–6 ml/kg (Anon. 1975)
LC50 values to fishes, mg/l	4 24hr, Carassius auratus (Anon.1975) 0.116 48hr, Oryzias latipes (MITI 1992)

601 • 1,3,5-Cycloheptatriene 544-25-2

Sumformula of the chemical	C7H8
State and appearance	Dark yellow liquid.
Molecular weight	92.14
Specific gravity (water=1)	0.89 at 20/4 °C
Melting point, °C	-79.5
Boiling point, °C	110–130 °C (Verschueren 1983)
Log octanol/water coefficient, log Pow	2.63 (Sangster 1989)
Henry's law constant, Pa x m³/mol	466 calc. (Yaws et al. 1991)
Chemical oxygen demand, g 02/g	2.3 5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.1 5 days (Bridie et al. 1979)

LD50 values to mammals in oral exposure, mg/kg	57	orl-rat (Anon. 1975)
LD50 values to mammals in non-oral exposure, mg/kg	442–884	mg/kg, dermal-rat (Anon. 1975)
LC50 values to fishes, mg/l	15	24hr, Carassius auratus (Anon. 1975)

602 • Cycloheptene

628-92-2

Molecular weight	96.17	
Specific gravity (water=1)	0.824	(Verschueren 1983)
Boiling point, °C	112–113 °C	(Verschueren 1983)
Effects on the reproduction of water organisms	Threshold conc. of cell multiplication inhibition of the protozoan Uronema parduczi Chatton-Lwoff: > 40 mg/l. (Bringmann & Kühn 1980b).	

603 • Cyclohexane

110-82-7

Synonyms	Hexahydrobenzene	
Sumformula of the chemical	C6H12	
State and appearance	Colourless, mobile liquid.	
Odour	Odour Index (O. I.) at 20 °C = 203000 In water: reduction of amenities: Threshold Odour Concentration: (T. O. C.) = 0.02 mg/l (Verschueren 1983)	
Molecular weight	84.16	
Specific gravity (water=1)	0.779	
Conversion factor, 1 ppm in air=	3.49	mg/m³ (Verschueren 1983)
Conversion factor, 1 mg/m³ in air=	0.29	ppm (Verschueren 1983)
Vapour pressure, mmHg	77	at 20 °C (Verschueren 1983)
Water solubility, mg/l	< 100 55 45	 at 20 °C at 15 °C
Melting point, °C	6.5	(MITI 1992)
Boiling point, °C	80.75	(MITI 1992)
Log octanol/water coefficient, log Pow	3.44	(Sangster 1989)
Henry's law constant, Pa x m³/mol	19530	calc. (Yaws et al. 1991)
Volatilization	Relative volatility (nBuAc=1) = 7.36	
Total degradation in water	Biodegradation: 0.6% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

Bioconcentration factor, fishes	31–102 8w, Cyprinus carpio, conc 0.1 mg/l 37–129 8w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	1297 orl-mus
Other information about mammals	Mouse: inhalation: LC50: -+18000 ppm, 1hr rabbit: inhalation: no effect level: 786 ppm, 10 weeks monkey: inhalation: no effect level: 1243 ppm, 6hr/day, 50days
Health effects	Man: irritating to the eyes and mucous membranes: 300 ppm. (Patty 1967)
Mutagenicity	Mutagenicity in the Salmonella test: none < 0.006 revertant colonies/nmol < 70 revertant colonies at 1000 mikro-g/plate (McCann et al. 1975)
LC50 values to fishes, mg/l	93 96hr, Pimephales promelas (Vincent et al. 1976) 32 96hr, Pimephales promelas 34 96hr, Pimephales promelas (Pickering & Henderson 1966) 93 96hr, Lake Superior, Pimephales promelas 117 96hr, reconst. water, Pimephales promelas (Mattson et al. 1976) 9 48hr, Oryzias latipes (MITI 1992)
Effects on the reproduction of water organisms	Threshold conc. of cell multiplication inhibition of the protozoa Uronema parduczi Chatton-Lwoff: > 50 mg/l (Bringmann & Kühn 1980b)
Other information about water organisms	Incubation with natural flora in the groundwater-in presence of the other components of high-octane gasoline (100 mikro-l/l). (Jamison et al. 1976) Mussel larvae (Mytilus edulis): 10-20% increase of growth rate at 1 to 100 ppm. (Verschueren 1983) Young Coho salmon: no significant mortalities up to 100 ppm after 96hrs in artificial sea water at 8 °C (Verschueren 1983)

604 • 1,2-Cyclohexanedicarboxylic acid 1687-30-5

Sumformula of the chemical	C8H12O4
Bioconcentration factor, fishes	< 0.2 6w, Cyprinus carpio, conc 0.5 mg/l < 2.0 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	> 500 48hr, Oryzias latipes (MITI 1992)

605 • 1,2-Cyclohexanedicarboxylic anhydride 85-42-7

Sumformula of the chemical	C8H10O3
EINECS-number	2016049
Melting point, °C	31–33 (MITI 1992)

Total degradation in water	Biodegradation: 1–6% by BOD (hydrolyzed to 1,2-Cyclohexanedicarboxylic acid) period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).

606 • Cyclohexanol

108-93-0

Synonyms	Hexahydrophenol Cyclohexylalcohol Hexalin Adronol Hydrophenol Hydralin	
Sumformula of the chemical	C6H12O	
Use	Solvent; intermediate (0.2%).	
State and appearance	Colourless liquid.	
Odour	Threshold Odour Concentration (T. O. C.): 0.21 mg/m³ = 0.05 ppm USSR: human reflex response: no response: 0.04 mg/m³ animal chronic exposure: no effect: 0.059 mg/m³ adverse effect: 0.61 mg/m³ (Stern 1968). In water: odour thresholds: detection: 3.5 mg/kg; 0.4 mg/kg (Cherkinski 1961).	
Molecular weight	100	
Specific gravity (water=1)	0.95	at 25/4 °C (Verschueren 1983)
Conversion factor, 1 ppm in air=	4.163	mg/m³ (Verschueren 1983)
Conversion factor, 1 mg/m³ in air=	0.244	ppm (Verschueren 1983)
Vapour pressure, mmHg	1 3.5	at 20 °C (Verschueren 1983) at 34 °C (Verschueren 1983)
Water solubility, mg/l	36000 37000	at 20 °C (MITI 1992)
Melting point, °C	22.6	(MITI 1992)
Boiling point, °C	161.1	(MITI 1992)
Log octanol/water coefficient, log Pow	1.2 1.23 1.23	(Anon. 1988) (Verschueren 1983) (Sangster 1989)
Henry's law constant, Pa x m³/mol	0.36	(Anon. 1988)
Volatilization	Relative volatility (nBuAc=1) = 0.05	

Mobility	Equilibrium distribution: *mass %* air 11.08 water 88.71 solid 0.21 (Anon. 1988).
Total degradation in water	Biodegradation: 94–99% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
LD50 values to mammals in oral exposure, mg/kg	2060 orl-rat 2200–2600 orl-rbt (Patty 1967)
Health effects	Man: irritation of eyes, nose and throat: 100 ppm, 3–5 min. (Patty 1967).
EC50 values to microorganism, mg/l	3105 Boidegradation inhibition (Vaishnav 1986)
LC50 values to fishes, mg/l	1100 96hr, Lepomis macrochirus 720 96hr, Menidia audens (Dawson et al. 1977) 1033 96hr, Pimephales promelas (Vincent et al. 1976) 704 96hr, Pimephales promelas (Veith et al. 1983)

C

607 • Cyclohexanone

108-94-1

Synonyms	Ketohexamethylene
Sumformula of the chemical	C6H10O
Use	Solvent for various insecticides.
Odour	Quality: sweet, sharp Hedonic tone: pleasant Threshold odour concentration absolute: 0.12 ppm 50% recognition: 0.12 ppm 100% recognition: 0.24 ppm Odour index 100% recognition: 10 958 (Hellman & Small 1974). USSR: human reflex response: no response: 0.06 mg/m³ animal chronic exposure: no effect: 0.042 mg/m³ adverse effect: 0.46 mg/m³ (Stern 1968). Odour index at 20 °C = 21900 (Verschueren 1983).
Molecular weight	98.15
Specific gravity (water=1)	0.95 at 20/4 °C (Verschueren 1983)
Conversion factor, 1 ppm in air=	4.08 mg/m³ (Verschueren 1983)
Conversion factor, 1 mg/m³ in air=	0.25 ppm (Verschueren 1983)
Vapour pressure, mmHg	4 at 20 °C (Verschueren 1983) 6.2 at 20 °C (Verschueren 1983)

C

Water solubility, mg/l	23000 20 °C 24000 31 °C 500 30 °C (MITI 1992)
Melting point, °C	-16.4 -26– -38 °C (Verschueren 1983) -45 (MITI 1992)
Boiling point, °C	156 (MITI 1992)
Log octanol/water coefficient, log Pow	0.81 (Verschueren 1983) 0.81 (Sangster 1989)
Volatilization	Relative volatility (nBuAc=1) = 0.22
Total degradation in water	Biodegradation: 87% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	1620 orl-rat
Other information about mammals	Rabbit: inhalation: no effect (liver alterration?): 190 ppm,10w rat: inhalation: survived: 4000 ppm, 4hr death: 8000 ppm, 8hr monkeys, rabbits: inhalation: no detectable effect: 190 ppm, 50x6hr slight eye irritation: 309 ppm, 50x6hr slightly increased mortality: 3082 ppm, 50x6hr (Patty 1967).
Health effects	Man: objectionable: 50 ppm satisfactory: < 25 ppm (Patty 1967).
Maximum longterm immission concentration in air for plants,mg/m³	10 VDI 2306
Maximum longterm immission concentration in air for plants,ppm	2 VDI 2306
Effects on microorganisms	Pseudomonas: still toxic at 500 mg/l (Meinck et al. 1970) Toxicity threshold (cell multiplication inhibition test): Pseudomonas putida: 180 mg/l (Bringmann & Kühn 1980a).
EC50 values to microorganism, mg/l	6969 Biodegradation inhibition (Vaishnav 1986)
LOEC values to algae, mg/l	52 rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to fishes, mg/l	527 96hr, Pimephales promelas (Veith et al. 1983)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): Microcystis aeruginosa 52 mg/l (Bringmann & Kühn 1976) Scenedesmus quadricauda 370 mg/l (Bringmann & Kühn 1980a) Entosiphon sulcatum 545 mg/l (Bringmann & Kühn 1980a) Uronema parduczi Chatton-Lwoff 280 mg/l (Bringmann & Kühn 1980b)

608 • Cyclohexanone oxime 100-64-1

Molecular weight	113.16	
Conversion factor, 1 ppm in air=	4.7	mg/m³ (Verschueren 1983)
Conversion factor, 1 mg/m³ in air=	0.21	ppm (Verschueren 1983)
Melting point, °C	90	
Boiling point, °C	206–210 °C (Verschueren 1983)	
Effects on microorganisms	Pseudomonas: toxic: 30 mg/l (Meinck et al. 1970)	
Other information about water organisms	Algae: Scenedesmus: toxic: 480 mg/l Protozoa: Colpoda: toxic: 60 mg/l Arthropoda: Daphnia: toxic: 120 mg/l (Meinck et al. 1970).	

609 • Cyclohexene 110-83-8

Sumformula of the chemical	C6H10	
Use	Solvent.	
Odour	Odour threshold: detection: 0.6 mg/m³ (Verschueren 1983)	
Molecular weight	82.14	
Specific gravity (water=1)	0.81	20/4 °C (Verschueren 1983)
Conversion factor, 1 ppm in air=	3.41	mg/m³ (Verschueren 1983)
Conversion factor, 1 mg/m³ in air=	0.29	ppm (Verschueren 1983)
Vapour pressure, mmHg	160	at 38 °C (Verschueren 1983)
Water solubility, mg/l	213	at 20 °C (Verschueren 1983)
Melting point, °C	-104	
Boiling point, °C	83	
Log octanol/water coefficient, log Pow	2.86	(Sangster 1989)
Henry's law constant, Pa x m³/mol	4569	calc. (Yaws et al. 1991)
Aerobic degradation in water	Biodegradation: cyclohexene →cyclohexanone (Ducan 1972)	
Effects on microorganisms	Pseudomonas putida: inhibition of cell multiplication starts at 17 mg/l (Bringmann & Kühn 1976)	
Other information about water organisms	Microcystis aeruginosa: inhibition of cell multiplication starts at > 160 mg/l (Bringmann & Kühn 1976) Threshold concentration of cell multiplication inhibition of the protozoa Uronema parduczi Chatton-Lwoff: > 50 mg/l (Bringmann & Kühn 1980b) Young Coho salmon: no significant mortalities up to 100 ppm after 96hr in artical sea water at 8 °C. (Verschueren 1983)	

C

610 • 4-Cyclohexene-1,2-dicarboxylic acid 88-98-2

Melting point, °C	100.8 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.2 6w, Cyprinus carpio, conc 2 mg/l < 2 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	600 48hr, Oryzias latipes (MITI 1992)

611 • 2-(1-Cyclohexene-1-yl)-1-cyclohexanone 1502-22-3

Synonyms	2-(1'-Cyclohexenyl)cyclohexanone
Water solubility, mg/l	300 (MITI 1992)
Melting point, °C	-78 (MITI 1992)
Boiling point, °C	265 160 mmHg (MITI 1992)
Log octanol/water coefficient, log Pow	3.17 (MITI 1992)
Total degradation in water	Biodegradation: 1% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	0.9–4.0 6w, Cyprinus carpio, conc 0.3 mg/l < 1.8–6.0 6w, Cyprinus carpio, conc 0.03 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	36.4 48hr, Oryzias latipes (MITI 1992)

612 • Cycloheximide 66-81-9

Sumformula of the chemical	C15H23NO4
EINECS-number	2006360
Water solubility, mg/l	> 1000 (MITI 1992)
Melting point, °C	107–120 (MITI 1992)
Log octanol/water coefficient, log Pow	0.85 (MITI 1992)

Total degradation in water	Biodegradation: 1% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.3 < 2.8	6w, Cyprinus carpio, conc 0.05 mg/l 6w, Cyprinus carpio, conc 0.005 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	1.6	48hr, Oryzias latipes (MITI 1992)

613 • Cyclohexyl amine 108-91-8

Synonyms	Aminocyclohexane Hexahydroaniline	
Sumformula of the chemical	C6H13N	
Molecular weight	99.2	
Specific gravity (water=1)	0.8191	at 20/4 °C (Verschueren 1983)
Conversion factor, 1 ppm in air=	4.06	mg/m³ (Verschueren 1983)
Conversion factor, 1 mg/m³ in air=	0.247	ppm (Verschueren 1983)
Melting point, °C	-18	
Boiling point, °C	134	
pKa	10.67	(Sangster 1989)
Log octanol/water coefficient, log Pow	1.49	(Sangster 1989)
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	156 400–800	orl-rat (Lewis & Sweet 1984) mg/kg orl-rat (5% soln) (Patty 1967)
LD50 values to mammals in non-oral exposure, mg/kg	277	skn-rbt (Lewis & Sweet 1984)
Effects on plants	In the laboratory, after 5 days of incubation in air from a 0.1% solution of cyclohexylamine (CHA), leaves of cucumber seedlings showed marginal, chlorotic areas, and some interveinal necrosis. When barley seeds were incubated in a tightly closed petri dish containing a small vial with 2 ml of pure CHA or a 10% solution, no germination was observed. When seeds were incubated in vapours from 1% and 0.1% solution of CHA germination was delayed for 48 hours (Pezet & Gindrat 1978).	
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): Pseudomonas putida: 420 mg/l (Bringmann & Kühn 1980a)	
EC50 values to algae, mg/l	20	96hr, rps, Selenastrum capricornutum (Calamari et al. 1982)
LOEC values to algae, mg/l	0.51 0.02	rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a) rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to crustaceans, mg/l	58	24hr, Daphnia magna (Calamari et al. 1982)

LC50 values to fishes, mg/l	44	96hr, Salmo gairdneri (Calamari et al. 1980)
	470	96hr, Branchydanio rerio
	58–95	48hr, Leuciscus idus (Wellens 1982)
Other information about water organisms	LOEC 0.6 mg/l, rpd, schr, Entosiphon sulcatum (Bringmann & Kühn 1980a).	
	Toxicity threshold (cell multiplication inhibition test):	
	Microcystis aeruginosa	0.02 mg/l (Bringmann & Kühn 1976)
	Scenedesmus quadricauda	0.51 mg/l (Bringmann & Kühn 1980a)
	Entosiphon sulcatum	0.6 mg/l (Bringmann & Kühn 1980a)
	Uronema parduczi Chatton-Lwoff	> 200 mg/l (Bringmann & Kühn 1980b)

614 • N-Cyclohexyl-N-nitrosohydroxylamine 4883-72-1

Sumformula of the chemical	C6H12O2N2	
Water solubility, mg/l	14000	(MITI 1992)
Melting point, °C	27	(MITI 1992)
Log octanol/water coefficient, log Pow	1.4	(MITI 1992)
Bioconcentration factor, fishes	< 0.4–1.7	6w, Cyprinus carpio, conc 0.4 mg/l
	< 4.2	6w, Cyprinus carpio, conc 0.04 mg/l (MITI 1992)
LC50 values to fishes, mg/l	34.7	48hr, Oryzias latipes (MITI 1992)

615 • N-Cyclohexyl-N-nitroso-hydroxylamine aluminium salt 40027-80-3

Water solubility, mg/l	< 100	(MITI 1992)
Melting point, °C	93.8–94.5	(MITI 1992)
Boiling point, °C	100	0.0001 mmHg (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD (hydrolyzed to N-Cyclohexyl-N-nitroso-hydroxyl amine) period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

616 • Cyclohexylacetate 622-45-7

Molecular weight	142.19	
Specific gravity (water=1)	1	
Melting point, °C	177	
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): Pseudomonas putida: 83 mg/l (Bringmann & Kühn 1980a).	
LOEC values to algae, mg/l	5.3	rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
	46	rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)

Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): Microcystis aeruginosa 46 mg/l (Bringmann & Kühn 1976) Scenedesmus quadricauda 5.3 mg/l (Bringmann & Kühn 1980a) Entosiphon sulcatum 120 mg/l (Bringmann & Kühn 1980a) Uronema parduczi Chatton-Lwoff > 400 mg/l (Bringmann & Kühn 1980b)

617 • 1,5-Cyclooctadiene 1552-12-1

Use	Resin intermediate.	
Molecular weight	108.18	
Specific gravity (water=1)	0.8803	at 20/20 °C (Verschueren 1983)
Vapour pressure, mmHg	5	at 20 °C (Verschueren 1983)
Melting point, °C	-69.5	
Boiling point, °C	150.9	
Chemical oxygen demand, g O2/g	2.62	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g O2/g	0.19	5 days (Bridie et al. 1979)
LD50 values to mammals in oral exposure, mg/kg	2700	orl-rat (Anon. 1975)
LC50 values to fishes, mg/l	14	96hr, Carassius auratus (Anon. 1975)

618 • Cyclopentane 287-92-3

Sumformula of the chemical	C5H10	
Use	Solvent for cellulose ethers.	
State and appearance	Colourless liquid.	
Molecular weight	70.14	
Specific gravity (water=1)	0.751	
Vapour pressure, mmHg	400	at 31 °C (Verschueren 1983)
Melting point, °C	-94	
Boiling point, °C	49.3	
Log octanol/water coefficient, log Pow	3	(Sangster 1989)
Henry's law constant, Pa x m^3/mol	19030	calc. (Yaws et al. 1991)
Other information about degradation	Incubation with natural flora in the groundwater – in presence of the other components of high-octane gasoline (100 micro-l/l) biodegradation: 0% after 192hr at 13 °C (initial conc 0.17 micro-l/l) (Jamison et al. 1976).	
Other information about water organisms	Young Coho salmon: no significant mortalities up to 100 ppm after 96hr in artificial sea water at 8 °C. (Verschueren 1983)	

619 • 1,3-Cyclopentanedisulfonyldifluoride 35944-73-1

Other information about mammals	ALD = 94.0 mg/kg, act, orl, deer mouse; LDfr = 75.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

620 • Cyclopentanol 96-41-3

Synonyms	Cyclopentyl alcohol Hydroxycyclopentane
Use	Perfume and pharmaceutical solvent; intermediate for dyes, pharmaceuticals and other organics.
Odour	Odour threshold: detection: 4200–8700 mg/m³ (Verschueren 1983)
Molecular weight	86.13
Specific gravity (water=1)	0.949
Melting point, °C	-19
Boiling point, °C	139–140 °C (Verschueren 1983)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): Pseudomonas putida: 250 mg/l (Bringmann & Kühn 1980a)
LOEC values to algae, mg/l	28 rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): Microcystis aeruginosa 28 mg/l (Bringmann & Kühn 1976) Scenedesmus quadricauda 255 mg/l (Bringmann & Kühn 1980a) Entosiphon sulcatum 290 mg/l (Bringmann & Kühn 1980a) Uronema parduczi Chatton-Lwoff> 800 mg/l (Bringmann & Kühn 1980b)

621 • Cyclopentanone 120-92-3

Synonyms	Ketopentamethylene
Use	Intermediate for pharmaceuticals, insecticides and rubber chemicals.
Odour	Odour threshold: detection: 31–1120 mg/m³. (Verschueren 1983)
Specific gravity (water=1)	0.943
Boiling point, °C	125–126 °C, 630 mm (Verschueren 1983)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): Pseudomonas putida: 175 mg/l. (Bringmann & Kühn 1980a).
LOEC values to algae, mg/l	63 rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
Other information about water organisms	LOEC 232 mg/l, rpd, schr, Entosiphon sulcatum (Bringmann & Kühn 1976). Toxicity threshold (cell multiplication inhibition test): Microcystis aeruginosa 63 mg/l (Bringmann & Kühn 1976) Scenedesmus quadricauda 1900 mg/l (Bringmann & Kühn 1980a) Entosiphon sulcatum 232 mg/l (Bringmann & Kühn 1980a) Uronema parduczi Chatton-Lwoff 1210 mg/l (Bringmann & Kühn 1980b)

622 • Cycocel Plus * (Chlormequat) 999-81-5

Active ingredients	Chlormequat chloride * 460 g/l
LC50 values to crustaceans, mg/l	80 96hr, 21 °C, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	1950 96hr, 10 °C, Alburnus alburnus (Linden et al. 1979)

623 • m-Cymene

535-77-3

Sumformula of the chemical	C10H14	
Water solubility, mg/l	< 10	(MITI 1992)
Boiling point, °C	176	(MITI 1992)
Log octanol/water coefficient, log Pow	5.11	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).	
Bioconcentration factor, fishes	362–636 357–718	8w, Cyprinus carpio, conc 0.02 mg/l 8w, Cyprinus carpio, conc 0.002 mg/l (MITI 1992)
LC50 values to fishes, mg/l	8.38	48hr, Oryzias latipes (MITI 1992)

624 • p-Cymene

99-87-6

Synonyms	1-Isopropyl-4-methylbenzene p-Isopropyltoluene	
Sumformula of the chemical	C10H14	
Molecular weight	134.24	
Water solubility, mg/l	23.35 5	25 °C (Banerjee et al. 1980) (MITI 1992)
Melting point, °C	-67.9	(Suntio et al. 1988)
Boiling point, °C	177	(MITI 1992)
Log octanol/water coefficient, log Pow	4.1 4.1 4.44	(Banerjee et al. 1980) (Sangster 1989) (MITI 1992)
Total degradation in water	Biodegradation: 83–95% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992). LD50 values to mammals in oral exposure, mg/kg: 4750	 orl-rat (Lewis & Sweet 1984)
LCLo values to mammals in inhalation exposure, ppm	5000	45 min., ihl-rat (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	> 316	orl-Agelaius phoeniceus (Schafer et al. 1983)
LC50 values to crustaceans, mg/l	6.5	48hr, Daphnia magna (LeBlanc 1980)

625 • Cypermethrin

52315-07-8

Synonyms	(RS)-α-cyano-3-phenoxybenzyl (1RS, 3RS, 1RS, 3SR)-3-(2,2-di-chloro-vinyl)-2,2-dimethylcyclopropanecarboxylate
Sumformula of the chemical	C22H19Cl2NO3
Use	Active ingredient in insecticides. Experimental photostable pyrethroid, insecticide.
Way to effect	Contact function
Molecular weight	416.32
Vapour pressure, mmHg	0.000000014 20 °C (KEMI 1990)
Water solubility, mg/l	0.041 room temperature 0.01–0.2 mg/l, 21 °C (KEMI 1990)
Melting point, °C	60–80 °C (KEMI 1990)
Log octanol/water coefficient, log Pow	4.47 (Verschueren 1983) 6.3 (KEMI 1990)
Mobility	The leaching of cypermethrin is slight. It can leach only few cm in soil. (KEMI 1990)
Hydrolysis in acid	In the hydrolysis studies it has noticed that cypermethin is more stabile in acid environment than in basic environment. (KEMI 1990)
Total degradation in soil	Degradation of cypermethrin in soil and water is happening with help of micro-organisms. It is little bit quicklier in the aerobic than anearobic conditions. Cypermethrin degrades mainly to CO2. (KEMI 1990)
Degradation and transformation products	cis, trans-3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropancarboxy late; 3-phenoxybenzylalcohol; 3-phenoxybenzylacid. (KEMI 1990)
LD50 values to mammals in oral exposure, mg/kg	251 orl-rat (Lewis & Sweet 1984) 160–300 mg/kg cis, orl-rat > 2000 trans, mg/kg, orl-rat (KEMI 1990)
LD50 values to mammals in non-oral exposure, mg/kg	> 2460 dr-rbt (KEMI 1990)
LC50 values to mammals in inhalation exposure, mg/m³	> 700 ihl-rat (KEMI 1990)
Effects on arthropods	Aedes stimulans; LC50: 0.000158 mg/l, 1d (Rice & White 1987) 0.000400 mg/l, 1d (Rice & White 1987) 0.000229 mg/l, 4d (Helson & Surgeoner 1986) 0.000570 mg/l, 4d (Helson & Surgeoner 1986) 0.00143 mg/l, 4d (Helson & Surgeoner 1986) Aedes vexans; LC50: 0.000072 mg/l, 3d (Helson & Surgeoner 1986) Culex pipiens; LC50: 0.000057 mg/l, 1d (Helson & Surgeoner 1986) 0.000175 mg/l, 1d (Helson & Surgeoner 1986) Culex restuans; LC50: 0.000073 mg/l, 1d (Helson & Surgeoner 1986) Culex sp.; LC50: 0.000045 mg/l, 1d (Helson & Surgeoner 1986) 0.000233 mg/l, 1d (Helson & Surgeoner 1986)

	Aedes sp.; 20 g/ha, 5d, Aedes stimulans; 10 g/ha, 6d, Culex sp.; 10 g/ha, 2d, lethal effect (100% mortality or 0% survival including algicidal and herbicidal effects) (Helson & Surgeoner 1986).	
LC50 values to crustaceans, mg/l	0.002	24hr, Daphnia magna (Nikunen et al. 1986)
	0.00001	96hr, Crangon septemspiosa
	0.00004	96hr, Homarus americanus
	0.0002	24hr, Asellus spp.
	0.0001	24hr, Gammarus pulex (McLeese et al. 1980)
LC50 values to fishes, mg/l	0.002	96hr, Salmo trutta m.lacustris
	0.0005	96hr, Salmo gairdneri (Pesticide Manual 1983)
	0.011	24hr, Salmo gairdneri, formulated prct
	0.055	24hr, Salmo gairdneri, technical grade (Coats & O'Donnell-Jeffery 1979)
	0.002	96hr, Salmo salar (McLeese et al. 1980)
Effects on the physiology of water organisms	Salmo gairdneri; 80 mg/kg; 0.08d, stress effect (Edwards et al. 1987).	

626 • 2,4-D

94-75-7

Synonyms	2,4-Dichlorophenoxyacetic acid	
Use	Active ingredient in herbicides.	
State and appearance	White powder	
Molecular weight	221.04	
Vapour pressure, mmHg	0.0000006	(McCall et al.1983)
	0.000008	20–25 °C (Weber et al. 1980)
Water solubility, mg/l	650	(Weber et al.1980)
Melting point, °C	136–140	
pKa	2.8	(Bovey & Young 1980, Weber et al. 1980)
Log octanol/water coefficient, log Pow	2.82	20 °C (Verschueren 1983)
Half-life in soil, days	7	(Li et al. 1990)
LD50 values to mammals in oral exposure, mg/kg	370	orl-rat
	100	orl-dog (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	1500	skn-rat
	1400	skn-rbt (Lewis & Sweet 1984)
LDLo values to mammals in oral exposure, mg/kg	800	orl-rbt (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	541	orl-ckn (Lewis & Sweet 1984)

Effects on plants	0.017 kg 2,4-D/ha reduced root weight of sugarbeets (Beta vulgaris) (Schweizer 1978). Incubation of segments of barley coleoptile and Sesbania exaltata hypocotyls in 1% sucrose containing 2 ppm 2,4-D inhibited protein synthesis by 15 and 4%, respectively (Mann et al. 1965). Aspen plants (Populus tremula) were grown in 0.000001 M 2,4-D solution → swelling of the stem base, time of survival ~25 days; 0.00001 M → epinastic curvatures, necrosis on the leaves, swelling of the stem base, time of survival 20 days (Eliasson 1963).	
LOEC values to algae, mg/l	50	Chlorococcus Isochrystis galbana Phaeodactylum tricornutum (Walsh 1972)
LC50 values to crustaceans, mg/l	< 1	Daphnia magna (Kenaga 1979)
	100	48hr, Daphnia magna (Crosby & Tucker 1966)
	> 40	act, Daphnia magna (Hashimoto & Nishiuchi 1981)
	363–389	48hr, Daphnia magna (Bogacka et al. 1983)
	36.4	48hr, Daphnia magna (Alexander et al. 1985)
	144.1	4d, Eudiaptomus gracilis (Presing & Ponyi 1986)
	> 40	48hr, Cyprinus carpio Carassius auratus (Hashimoto & Nishiuchi 1981)
	2630	48hr, Lebistes reticulatus (Bogacka et al. 1983)
	1	48hr, Cyprinus carpio (Nishiuchi & Hashimoto 1967)
	320 263 358	96hr, Pimephales promelas 96hr, Lepomis macrochirus 96hr, Salmo gairdneri (Alexander et al. 1985)
LC50 values to fishes, mg/l	1.1 0.9	48hr, Salmo gairdneri 48hr, Lepomis macrochirus (Edwards 1977)
	0.39 2.1 5	act, Lepomis macrochirus act, Salmo gairdneri act, Pimephales promelas (Kenaga 1979)
	96 71 12.9	96hr, Cyprinus carpio 96hr, Poecilia reticulata 48hr, embryo, Alburnus alburnus (Biro 1979)
	5.1–35 3.8 5.6	96hr, Cyprinus carpio 96hr, Labeo boga 96hr, Rasbora neilgeriensis (Vardia & Durve 1981)
	11	23 days, embryo, Salmo gairdneri (Birge et al. 1979)
	250	24hr, Salmo gairdneri (Alabaster 1969)
LOEC values to fishes, mg/l	1.5	chr, Pimephales promelas (Mount & Stephan 1967)
NOEC values to fishes, mg/l	0.3	chr, Pimephales promelas (Mount & Stephan 1967)
	50 10	srv, act, Salmo gairdneri srv, act, Oncorhynchus kisutch (Meehan et al. 1974)

627 • 2,4-D butoxyethanol ester 1929-73-3

Synonyms	2,4-D butoxyethyl ester 2,4-D(BEE) 2,4-Dichlorophenoxyacetic acid, butoxy-ethanol ester	
State and appearance	Amber liquid.	
LD50 values to mammals in oral exposure, mg/kg	940	orl-rat (Verschueren 1983)
LD50 values to mammals in non-oral exposure, mg/kg	4000	skn-rbt (Verschueren 1983)
LOEC values to algae, mg/l	75	rpd, schr, Chlorococcum sp. Isochrystis galbana Dunaliella tertiolecta (Walsh 1972)
LC50 values to crustaceans, mg/l	1.8 1.4 5.6	48hr, Cypridopsis vidua 48hr, Palaemonetes kadiakensis 48hr, Daphnia magna (Sanders 1970)
	0.44	96hr, Gammarus lacustris (Sanders 1969)
LC50 values to fishes, mg/l	1.5	96hr, Pimephales promelas (Mount & Stephan 1967)

628 • 2,4-D butyl ester 94-80-4

Synonyms	2,4-D(BE) Butyl dichlorophenoxyacetate	
Molecular weight	277.16	
LD50 values to mammals in oral exposure, mg/kg	995 780	orl-rat orl-cat (Lewis & Sweet 1984)
Effects on plants	1.12 kg mixed butyl ester of 2,4-D/ha was applied with a sprayer → 1) decrease in number of Canada thistle (Circium arvense) shoots emerging 1 yr following a single herbicide treatment and a delay in budding and flowering, 2) reduction in timothy (Pleum pratense) seed production (postemergence application) (Gallagher & Vanden Born 1976).	
LC50 values to fishes, mg/l	0.6 0.49	96hr, Salvelinus namaycush 96hr, Salmo clarki (Woodward & Mayer 1978)
	0.78	96hr, Salmo clarki (Woodward 1982)
NOEC values to fishes, mg/l	1	srv, act, Salmo gairdneri Oncorhynchus kisutch (Meehan et al. 1974)

629 • 2,4-D dimethylaminesalt 2008-39-1

LC50 values to fish, mg/l	335 155 168 236	96hr, Pimephales promelas 96hr, Ictalurus punctatus 96hr, Lepomis macrochirus 96hr, Micropterus dolomieui (Johnson & Finley 1980)
LOEC values to fishes, mg/l	1	bhr, act, Salmo gairdneri (Folmar 1978)

630 • 2,4-D isooctyl ester 25168-26-7

Synonyms	2,4-Dichlorophenoxyacetic acid isooctylester 2,4-D(IOE)	
State and appearance	Dark liquid.	
Molecular weight	333.28	
Water solubility, mg/l	10	
Boiling point, °C	317	
LC50 values to crustaceans, mg/l	2.4 2.4	96hr, Gammarus lacustris (Sanders 1969) 67%, 96hr, Gammarus fasciatus (Johnson & Finley 1980)
LC50 values to fishes, mg/l	> 50	Salmo clarci (Woodward 1982)
NOEC values to fishes, mg/l	10 1	srv, act, Salmo gairdneri srv, act, Oncorhynchus kisutch

631 • 2,4-D sodium salt 2702-72-9

Synonyms	2,4-Dichlorophenoxyacetic acid, sodium salt	
LC50 values to crustaceans, mg/l	68.6–173.4	4d, Eudiaptomus gracilis (Presing & Ponyi 1986)

632 • Dacthal 1861-32-1

Synonyms	Dimethyltetrachloroterephthalate Chlorthaldimethyl DAC 893 Fatal Chlorthalmethyl DCPA	
Use	Selective preemergence herbicide.	
State and appearance	White crystals.	
Vapour pressure, mmHg	< 0.5 at 40 °C (Verschueren 1983)	
Water solubility, mg/l	0.5	
Melting point, °C	156	
LD50 values to mammals in oral exposure, mg/kg	> 3000	orl-rat, act (Anon. 1976)
Effects on plants	DCPA at 22 kg ai/ha gave complete control of crabgrass (Callahan 1980).	
LC50 values to fishes, mg/l	700	48hr, Lepomis macrochirus (Hughes & Davis 1964)

633 • 2,4-DB 94-82-6

Synonyms	4-(2,4-Dichlorophenoxy)butyric acid
Use	Herbicide.
Molecular weight	249.1
Total degradation in soil	Biodegradation: 11 days for ring cleavage in soil suspension (Verschueren 1983).

LD50 values to mammals in oral exposure, mg/kg	700	orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	800	skn-rat (Lewis & Sweet 1984)
Effects on plants	Application of 2,4-DB ester with a sprayer at 0.14 kg/ha caused slight damage to sainfoin seedlings (Onobrychis viciaefolia) grown in the greenhouse (Waddington 1978).	
LC50 values to crustaceans, mg/l	5	96hr, Daphnia magna (Knapek & Lakola 1974)
LC50 values to fishes, mg/l	6.3	96hr, Cyprinus carpio (Knapek & Lakola 1974)

634 • DDD

72-54-8

Synonyms	Tetrachlorodiphenylethane 4,4-DDD Dichlorodiphenyldichloroethane 2,2-Bis(p-chlorophenyl)-1,1-dichloroethane
Use	Nonsystemic contact and stomach insecticide. The technical grade contains related compounds in small amounts, the greatest being being the o, p'-isomer.
Molecular weight	320.1
Water solubility, mg/l	0.16 24 °C
Melting point, °C	112
Total degradation in water	100% of original compound found after 8 weeks (river water in a sealed glass, initial conc. 10 µg/l (Verschueren 1983).
Other information about degradation	Persistence in river water in a sealed glass jar under sunlight and artificial fluorescent light – initial conc. 0.01 mg/l *% of original compound found* after: 1hr 100; 1wk 100; 2wk 100; 4wk 100; 8wk 100 (Eichelberger & Lichtenberg 1971).
Bioconcentration factor, fishes	2710 (Verschueren 1983)
Bioconcentration factor, mollusca	4460–9120 (Verschueren 1983)
Bioconcentration factoralgae	6210 (Verschueren 1983)
LD50 values to mammals in oral exposure, mg/kg	113 orl-rat (Lewis & Sweet 1984) 3400 orl-rat (Anon. 1976)
LD50 values to mammals in non-oral exposure, mg/kg	1200 skn-rbt (Lewis & Sweet 1984) 3400 ukn-rat (Virtanen & Nuuja 1987)
Carcinogenicity	NCI carcinogenesis bioassay completed: results indefinite, rat; results negative, mus (Lewis & Sweet 1984).
Effects on arthropods	LC50, 0.38 mg/l, 96hr, Pteronarcys californica (Sanders & Cope 1968)

D

LC50 values to crustaceans, mg/l	0.0032	48hr, Daphnia magna (Sanders & Cope 1966)
	0.00064	96hr, Gammarus lacustris (Sanders 1972)
	0.00086	96hr, Gammarus fasciatus
	0.00068	96hr, Palaemonetes kadiakensis
	0.01	96hr, Asellus breviacaudus (Sanders 1972)
	0.0045	48hr, Simocephalus serrulatus
	0.0032	48hr, Daphnia pulex (Sanders & Cope 1966)

635 • DDE

72-55-9

Synonyms	p, p'-DDE Dichlorodiphenyldichloroethylene
Use	Military product, DDT impurity.
Water solubility, mg/l	0.04 at 20 °C (Verschueren 1983) 0.065 at 24 °C (Verschueren 1983)
Log octanol/water coefficient, log Pow	4.28 (Verschueren 1983) 5.69 (Verschueren 1983) 5.69 (Mackay 1982)
Other information about degradation	Degrades further to DDA (bis(chlorophenyl)acetic acid) by loss of to more molecules HCl(Anon. 1976). Persistence in river water in a sealed glass jar under sunlight artificial fluorescent light-initial conc. 0.01 mg/l: *% of original compound found* after: 1hr 100; 1wk 100; 2wk 100; 4wk 100; 8wk 100 (Eichelberger & Lichtenberg 1971).
Bioconcentration factor, fishes	8450 Cyprinus carpio (Miyamoto et al. 1979) 12037 Gambusia affinis (Metcalf et al. 1975)
Bioconcentration factor, algae	2720 (Miyamoto et al. 1979) 11251 Oedogonium cardiacum (Metcalf et al. 1979)
Bioconcentration factor, other organisms	13700 Cipangopaludina japonica Martens (Miyamoto et al. 1979) 36342 Physa 59390 Culex pipiens quinquefasciatus (Metcalf et al. 1975)
Carcinogenicity	Positive.
Mutagenicity	Mutagenicity in the Salmonella test: negative < 0.004 revertant colonies/nmol < 70 revertant colonies at 5000 mikro-g/plate (McCann et al. 1975).
Other information	Agricultural runoff degradation of DDT, lab use. (Verschueren 1983).

636 • DDM

101-77-9

Synonyms	p, p'-Methylenedianiline 4,4'-Diaminodiphenylmethane
Known impurities	2,4'-methyleneaniline: 4%, technical grade.

Use	In preparation of isocyanates and polyisocyanates; an epoxy hardening agent: a raw material in the production of polyurethane elastomers; in the rubber industry; a curative for neoprene; an anti-frosting agent (anti-oxidant) in footwear; a raw material in the preparation of poly(amide-imide)resins (used in magnet wire enamels).
Molecular weight	198.26
Water solubility, mg/l	1000 (MITI 1992)
Melting point, °C	93 (MITI 1992)
Boiling point, °C	231 at 11 mm (Verschueren 1983) 232 9 mmHg (MITI 1992)
Log octanol/water coefficient, log Pow	1.64 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	0–14 6w, Cyprinus carpio, conc 0.2 mg/l < 3.1–15 6w, Cyprinus carpio, conc 0.02 mg/l, (MITI 1992)
LD50 values to mammals in oral exposure, mg/kg	120–250 orl-rat (Verschueren 1983)
Effects on the physiology of mammals	16 rats: 4–5 doses of 20 mg DDM by stomach tube over 8 months: after 18 months: 1 rat developed a hepatoma and a heamangioma-like tumor of the kidney after 24 months: 1 rat showed an adenocarcinoma of the uterus 50 rats: 50% developed tumors (4 hepatomas) compared with 26% of a control group 50 rat: 50% developed tumors (4 hepatomas) compared with 26% of a control group 48 rats: intragastric doses 5 times weekly: all developed liver cirrhosis, four developed hepatomas (2 benign) and others miscellaneous tumors (Verschueren 1983).
Health effects	Hepatotoxic in humans: no reported human cancers. (Verschueren 1983)
Effects on microorganisms	Pseudomonas: toxic: 15 mg/l (Meinck et al. 1970)
LC50 values to fishes, mg/l	32 48hr, Oryzias latipes (MITI 1992)
Other information about water organisms	Scenedesmus: toxic: 30 mg/l Colpoda: toxic: 124 mg/l Daphnia: toxic: 0.25 mg/l (Meinck et al. 1970).

637 • DDT

50-29-3

Synonyms	Dichloro diphenyl trichloroethane p, p'-DDT 1,1,1-Trichloro-2,2-bis(p-chlorophenyl)ethane 1,1,1-Trichloro-2,2-bis-(4-chlorophenyl)ethane
Sumformula of the chemical	C14H9Cl5
Use ceased in year	1977
Use	Insecticide, nematocide. Mainly in tropical devoloping countries.
Odour	Odour threshold: detection: 0.35 mg/kg water (Sigworth 1964)
Molecular weight	354.48

Density, kg/m³	1550 20 °C
Vapour pressure, mmHg	0.00000019, 20 °C
Water solubility, mg/l	0.0031–0.0034, 25 °C < 1 (MITI 1992)
Melting point, °C	108 (MITI 1992)
Boiling point, °C	260
Log octanol/water coefficient, log Pow	6.19 (Anon. 1986, Anon.1988) 6.19 (Schwarzenbach & Westall 1981) 6.28 (Anon. 1986) 6.19 at 20 °C (Verschueren 1983) 5.75 (Mackay 1982) 6.38 (MITI 1992)
Log organic C/water coefficient, log Pcw	5.14 exptl (Schwarzenbach & Westall 1981) 4.95 calcd (Schwarzenbach & Westall 1981)
Henry's law constant, Pa x m³/mol	2.7 (Anon. 1988) 3.94 (Anon. 1989)
Mobility	Equilibrium distribution: *mass %* air 0.40 water 0.42 solid 99.18 (Anon. 1988).
Photochemical degradation in air	Degradation very slow in sunlight: 34% in 7 days (> 290 nm) (Gäb et al. 1975).
Photochemical degradation in water	Permanent in sunlight (in river water) for 8 weeks. In tropical conditions, photochemical degradation is faster (Eichelberger & Lichtenberg 1971). Photooxidation by u. v. lihgt in aqueous medium at 90–95 °C: time for the formation of CO2 (% of theoretical) 25%: 25.9hr 50%: 66.5hr 75%: 120.0hr (Verschueren 1983).
Half-life in soil, days	3837 (Li et al. 1990) 1086–3620 3–10 years (Ray & Trieff 1980)
Half-life in water, days	3.08 = 73.9hr, calculated,25 °C,1 m depth (Verschueren 1983)
Aerobic degradation in water	Permanent in static bottle test (28 d) (Tabak et al. 1981); although very slow degradation to DDD (Kobayashi & Rittmann 1982).
Anaerobic degradation in water	Anaerobic degradation to DDD (Guenzi & Beard 1968).
Total degradation in soil	75–100% disappearance from soils: 4–30 years (Edwards 1966).
Total degradation in water	In river water: 100% of original compound found after 8 weeks (Verschueren 1983). Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Other information about degradation	Degradation products of special interest: DDE, DDD, 3-methylsulfonyl-DDE (very toxic in mammals) (Lund et al. 1988).

Other information about metabolism	A metabolite 3-methylsulfonyl-DDE is found in seals. The chemical is persistent and strongly toxic after metabolic activation (Jensen & Jansson 1976, Lund et al. 1988). DDT induces MFO-enxymes in liver in birds and mammals (WHO 1979).
Bioconcentration factor, mammals	37000000 sea water/dolphin (Virtanen & Nuuja 1987)
Bioconcentration factor, fishes	29400 p, p'-DDT, 32d, Pimephales 51000 p, p'-DDE, 32d, Pimephales (Veith et al. 1979) 2390 Cyprinus carpio 200 Salmo (Verschueren 1983) 5100–24400 10w, Cyprinus carpio, conc 0.001 mg/l 6080–25900 10w, Cyprinus carpio, conc 0.0001 mg/l (MITI 1992)
Bioconcentration factor, mollusca	700–70000 (Verschueren 1983) 70000 oyster (Weber 1977) 15000 sum of DDT (Verschueren 1983)
Bioconcentration factor crustaceans	12100 sea water/zoopl. (Virtanen & Nuuja 1987) 20000 Daphnia (Kenaga & Goring 1980)
Bioconcentration factor, algae	4720–80000
Bioconcentration factor, other organisms	80000 Amphidinium (Cox 1970)
Other information about bioaccumulation	Confirmed to be accumulated on a high level (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	87 orl-rat 200 orl-mky (Lewis & Sweet 1984) 113 orl-rat (Lewis & Tatken 1980)
LD50 values to mammals in non-oral exposure, mg/kg	300 skn-rbt 1931 skn-rat (Lewis & Sweet 1984) 200 ukn-rat (Virtanen & Nuuja 1987)
Other information about mammals	3-methylsulfonyl-DDE: mouse, acute injuries in adrenal glands (Lund et al. 1988).
Health effects	Man, 0.5 mg/kg, per day, during 21 months, no harmful effects (Martin 1968).
Carcinogenicity	NCI carcinogenesis bioassay completed: results negative, mus, rat (Lewis & Sweet 1984). No carcinogenic effects in humans after 1300 months, 10–20 years (Rippen 1988).
Mutagenicity	Negative in the Ames test (van Dijk & van de Vorde 1976).
LDLo values to birds in oral exposure, mg/kg	300 orl-ckn (Lewis & Sweet 1984)
Effects on the reproduction of birds	Ring-dove, DDE induces thinning of the eggshell and impaired reproduction (Moriarty 1988).
EC50 values to algae, mg/l	0.1 7d, Skeletonema (Pomeroy et al. 1980)

D

LOEC values to algae, mg/l	0.001	rpd, phy, chr, Chlorella fusca (Goulding et al. 1984)
	0.01	pht, act, 4hr, Dunaliella euchlora
	0.01	pht, act, 4hr, Skeletonema costatum (Derby & Ruber 1971)
LC50 values to crustaceans, mg/l	0.00036	48hr, Daphnia pulex (Sanders & Cope 1966)
	0.00036	48hr, Daphnia magna (Sanders & Cope 1966, Frear & Boyd 1967)
	0.048	24hr, Macrobrachium kistensis (Fawade et al. 1983)
	0.003	96hr, Daphnia magna (Knapek & Lakola 1974)
	0.001	48hr, Daphnia magna (Randall et al. 1979)
	0.001	act, Daphnia magna (Kenaga 1979)
	0.0008	96hr, Gammarus fasciatus
	0.00024	96hr, Orconectes nais (Sanders 1972)
	0.00148	48hr, Daphnia pulex (Priester 1966)
	> 40	act, Daphnia pulex (Hashimoto & Nishiuchi 1981)
	3.5	act, Daphnia pulex (Nishiuchi & Hashimoto 1967)
	0.0086	1d, Macrobrachium lamarrei
	0.0061	2d, Macrobrachium lamarrei
	0.0047	3d, Macrobrachium lamarrei (Mary et al. 1986)
	0.03	96hr, Nitocra (Linden et al. 1979)
	0.56	4d, Bara telphusa cunicularis (Rao & Nagabhushanam 1987)
	0.004	96hr, Asellus, 21 °C
	0.001	96hr, Gammarus lacustris, 21 °C
	0.0023	96hr, Palaemonetes, 21 °C
	0.00018	96hr, juvenile, Orconectes, 21 °C (Johnson & Finley 1980)
	0.0023	96hr, Palaemonetes kadiakensis
	0.004	96hr, Asellus brevicaudus (Sanders 1972)
	0.0025	48hr, Simocephalus serrulatus (Sanders & Cope 1966)
EC50 values to crustaceans, mg/l	0.0004–0.001	48hr, Daphnia pulex (Shapiro 1974)
	1.1	2d, mbt, Daphnia pulex (Passino & Smith 1987)
	0.0047	48hr, Daphnia magna, first instar, 15 °C
	0.015	48hr, Cypridopsis, 21 °C (Johnson & Finley 1980)
LC50 values to fishes, mg/l	0.00026	15d, Salmo gairdneri (Verschueren 1983)
	0.007	96hr, Salmo gairdneri
	0.002	96hr, Salmo trutta
	0.009	96hr, Perca fluviatilis (Macek & McAllister 1970)
	0.122	48hr, Aplocheilus lineatus
	2.28	48hr, Macrobodus cupatus (Jacob et al. 1982)
	0.151	96hr, Cyprinus carpio (Singh et al. 1981)
	0.54	96hr, Cyprinus carpio
	0.046	96hr, Salmo gairdneri (Knapek & Lakola 1974)

	0.003	96hr, Lepomis macrochirus (Randall et al. 1979)
	0.068	48hr, Carassius auratus (Hashimoto & Nishiuchi 1981)
	0.11	48hr, Cyprinus carpio (Nishiuchi & Hashimoto 1967)
	0.005 0.019 0.002	act, Lepomis macrochirus act, Pimephales promelas act, Salmo gairdneri (Kenaga 1979)
	0.0004	96hr, Medinia medinia (Lowe 1967)
	0.0058	96hr, Pimephales promelas (Priester 1966)
	0.35	4d, Cyprinus carpio (Kulshrestha & Arora 1986)
	0.004 0.0087 0.0027 0.0122 0.0215 0.0086 0.0015 0.009	96hr, Oncorhynchus kisutch, 13 °C 96hr, Salmo gairdneri, 13 °C 96hr, Esox lucius, 13 °C 96hr, Pimephales promelas, 18 °C 96hr, Ictalurus punctatus, 18 °C 96hr, Lepomis macrochirus, 18 °C 96hr, Micropterus salmoides, 18 °C 96hr, Perca flavescens, 18 °C (Johnson & Finley 1980)
	0.0335	48hr, Oryzias latipes (MITI 1992)
LOEC values to fishes, mg/l	0.002	srv, rpd, schr, Pimephales promelas (Järvinen et al. 1977)
NOEC values to fishes, mg/l	0.0005	srv, rdp, schr, Pimephales promelas (Järvinen et al. 1977)
Effects on the physiology of water organisms	Cyprinus carpio; 0.01 mg/100g/day; 10d, biochemical effect (change in physio-chemical process including glycogen uptake, cholesterol levels and lipid analysis) (Kobayashi et al. 1987). Tilapia mossambica; 0.001 mg/l, 20d, histological effect (presence of physical damage to tissues) (Shukla & Pandey 1986).	
Other information about water organisms	LC50, 24hr, Chironomus, 0.0047 mg/l (Estenik & Collins 1979). LC50, 10d, 3.98 mg/l, Phagocata gracilis (Bonner & Wells 1987). LC50, 96hr, 0.007 mg/l, 15 °C, Pteronarcys, second year class; LC50, 96hr, 0.0012 mg/l, 15 °C, Isoperla, juvenile; LC50, 96hr, 0.0074, 15 °C, Chaoborus, juvenile (Johnson & Finley 1980). The p, p'-isomer appears to be more toxic than the o, p-isomer to invertebrates. DDE is one of the primary metabolites of DDT in invertebrates and produces biological effects similar to those of the parent compound. DDT rapidly accumulates in invertebrates to several thousand times the exposure level in concentrations as low as 80 ng/l. The residue half-life was 7 days in Daphnia. A 60% reproductive impairment was observed in Daphnia at 0.100 mg/l. No difference in toxicity was noted between hard and soft water. Although isomers tested were toxic to rainbow trout sac fry, the more polar compounds appeared more toxic than the less polar ones. DDT detrimentally altered several physiological characteristics, including normal ratios of serum amino acids, thyroid activity, and the ability to withstand stress. Food seems to be more important than water as a source of body residues. Although DDT was not observed to affect gonad maturation, the mortality of fry produced by treated parents was high, especially during the terminal stages of yolk absorption (Johnson & Finley 1980).	
Other information	The toxicity increases when the hardness of water increases (Bergling & Dave 1984).	

D

638 • Decabromodiphenyl 13654-09-6

Melting point, °C	375	(MITI 1992)
Total degradation in water	Biodegradation: 0.8% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).	
Bioconcentration factor, fishes	0.6–5.4 < 4	6w, Cyprinus carpio, conc 0.15 mg/l 6w, Cyprinus carpio, conc 0.015 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	250	48hr, Oryzias latipes (MITI 1992)

639 • Decabromodiphenyl ether 1163-19-5

Water solubility, mg/l	0.02	(MITI 1992)
Melting point, °C	285	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 5 < 50	6w, Cyprinus carpio, conc 0.06 mg/l 6w, Cyprinus carpio, conc 0.006 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LOEC values to fishes, mg/l	> 500	48hr, Oryzias latipes (MITI 1992)

640 • Decahydronaphthalene 91-17-8

Sumformula of the chemical	C10H18	
EINECS-number	2020469	
Water solubility, mg/l	< 10	(MITI 1992)
Melting point, °C	-43 -30.4	cis- (MITI 1992) trans- (MITI 1992)
Boiling point, °C	194.6 185.5	cis- (MITI 1992) trans- (MITI 1992)
Total degradation in water	Biodegradation: 1–3% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

Bioconcentration factor, fishes	839–2380 8w, Cyprinus carpio, conc 0.0021 mg/l cis- 1170–3050 8w, Cyprinus carpio, conc 0.0028 mg/l trans- 1290–2400 8w, Cyprinus carpio, conc 0.00021 mg/l cis- 1300–2510 8w, Cyprinus carpio, conc 0.00028 mg/l trans- (MITI 1992)
LC50 values to fishes, mg/l	1.84 48hr, Oryzias latipes (MITI 1992)

641• Decalin

493-01-6 * cis-decalin
493-02-7 * trans-decalin

Use	Solvent for oils, fats, waxes, resins, rubbers etc.
Odour	Threshold odour concentration: 0.1 mg/l. (Verschueren 1983)
Molecular weight	138.25
Specific gravity (water=1)	0.8967 at 20 °C
Conversion factor, 1 ppm in air=	5.75 mg/m³ (Verschueren 1983)
Conversion factor, 1 mg/m³ in air=	0.17 ppm (Verschueren 1983)
Vapour pressure, mmHg	1 at 23 °C
Melting point, °C	-43 cis-decalin -31 trans-decalin
Boiling point, °C	194 cis-decalin 186 trans-decalin
Other information about degradation	Degradation in seawater by oil oxidizing micro-organisms: 13.6% breakdown after 21 days at 22 °C in stoppered bottles containing a 1000 ppm mixture of alkanes, cycloalkanes and aromatics (McKenzie & Hughes 1976).
Other information about mammals	Rat: inhalation: no effect level: 200 ppm, 20x6hr (Gage 1970) guinea pig: inhalation: 1/3: 319 ppm, 8hr/day, 1d 2/3: 319 ppm, 8hr/day, 21d 3/3: 319 ppm, 8hr/day, 23d (Summer 1971).
Effects on the physiology of water organisms	Mussel larvae (Mytilus edulis): +/- 20% reduction of growth rate at 10 ppm and 50 ppm +/- 5% reduction of growth rate at 100 ppm (Verschueren 1983).

642 • Decamethrin

52820-00-5

Synonyms	Deltamethrin Cyclopropanecarboxylic acid,3-(2,2-dibromoethenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester (S)-α-Cyano-3-phenoxybenzyl-(1R,3R)-3-(2,2-dibromovinyl)-2,2-dimethylcyclopropanecarboxylate
Sumformula of the chemical	C22H19Br2NO3 52918-63-5 * (1R-(1-α(S*),3-α))-
Use	Active ingredient in insecticides.
Molecular weight	505.24
Vapour pressure, mmHg	0.000000015, at 25 °C (KEMI 1990)
Water solubility, mg/l	< 0.002 mg/l, 20 °C (KEMI 1990)

Melting point, °C	98–102 °C (KEMI 1990)
Log octanol/water coefficient, log Pow	5.4 (KEMI 1990)
Mobility	The leaching behaviour of deltametrin was studied in different soil types. Deltametrin didn't leach or only a few. The transformationproducts were leaching more than deltametrin. Rf-values for transformation products were 0.1–0.7 (KEMI 1990).
Total degradation in soil	Deltametrin was degraded by microorganisms. Degradation was quicklier in acidic and/or granular soils with low contents of organic carbon. Half-lives of deltametrin were 11–72 days, depends on temperature (KEMI 1990).
Other information about bioaccumulation	BCF-value for fish was determined 972 for viscera and 144 for hole fish (KEMI 1990).
LD50 values to mammals in oral exposure, mg/kg	31 orl-rat (Lewis & Sweet 1984) 80 52820-00-5, orl-rat (Sweet 1987) 3450 52918-63-5, orl-mus (Sweet 1987) 30 52918-63-5, orl-rat (Sweet 1987) 77 52918-63-5, orl-rat (KEMI 1990)
LD50 values to mammals in non-oral exposure, mg/kg	> 2940 52918-63-5, idr-rbt (KEMI 1990)
LC50 values to mammals in inhalation exposure, mg/m³	785 2hr, ihl-rat (Lewis & Sweet 1984) 600 6hr, 52918-63-5, ihl-rat (KEMI 1990)
LDLo values to mammals in non-oral exposure, mg/kg	6 52820-00-5, ivn-mus (Sweet 1987) 0.08 52918-63-5, icb-mus (Sweet 1987) 1 52918-63-5, ivn-rat (Sweet 1987)
TDLo values to mammals in oral exposure, mg/kg	30 52918-63-5, orl-mus, 7–16d preg, specific developmental abnormalities 70 52918-63-5, orl-rat, 7–20d preg, effects on newborn (Sweet 1987)
Other information about mammals	In 3 months studies with rat and dog it was found effects in reflexs and in moving. NOEL: 1.0 mg/kg/day (KEMI 1990).
Carcinogenicity	In the chronic toxicity studies the only effect was degreasing bodyweight with rat and mouse. Anything about cancer wasn't observed. NOEL: 2.5 mg/kg/day (rat) and 13 mg/kg/day (mouse) (KEMI 1990).
Mutagenicity	Cytogenetic analysis: fish-multiple; 100 nl/l, CAS 52918-63-5 (Sweet 1987).
Other information about birds	Acute and subacute toxicity for birds was low and moderate, respectively. The toxicity was biggest for duck. LD50:> 4000 mg/kg (duck); LC50:> 4640 mg/kg feed (duck) (KEMI 1990).
Effects on bees	Deltametrin has found to be very high toxicity for bees at laboratory. LD50 (acute contact) 0.047–0.067 µg/bee (KEMI 1990).
LC50 values to fishes, mg/l	0.0005 48hr, Salmo gairdneri, 0.0006 48hr, Cyprinodon macularis, 0.001 48hr, Gambusia affinis 0.008 48hr, Tilapia mossambica 52918-63-5 (Mulla et al. 1978) 0.01–0.001 fishes, act 52918-63-5 (Pesticide Manual 1983)
Other information about water organisms	Deltametrin has found to be very high acute toxicity for fish in the laboratory studies. LC50: 0.0004–0.002 mg/l, different fishes, 50–96hr (KEMI 1990). Deltametrin has found to be very high toxicity for Daphnia. LC50: 0.005 mg/l (KEMI 1990).

643 • n-Decane

124-18-5

Use	Organic synthesis; solvent; standardized hydrocarbon; jet fuel reseach; mfg. paraffin product; rubber industry; paper prosessing industry; constituent in polyolefin manufacturing wastes.	
Odour	Threshold odour concentration : 10 mg/l (Zoeteman et al. 1971)	
Molecular weight	142.28	
Specific gravity (water=1)	0.73	
Vapour pressure, mmHg	2.7	at 20 °C (Verschueren 1983)
Water solubility, mg/l	0.009 0.087	20 °C, in distilled water 20 °C, in salt water (Verschueren 1983)
Melting point, °C	-32—30 °C (Verschueren 1983)	
Boiling point, °C	173–174 °C (Verschueren 1983)	
Log octanol/water coefficient, log Pow	6.25	(Sangster 1989)
Other information about degradation	Degradation in seawater by oil-oxidizing micro-organisms: 100% breakdown after 21 days at 22 °C in stoppered bottles containg a 1000 ppm mixture of alkanes, cyclo-alkanes and aromatics (McKenzie & Hughes 1976).	
LC50 values to crustaceans, mg/l	18	48hr, Daphnia magna (LeBlanc 1980)
Effects on the physiology of water organisms	Mussel larvae (Mytilus edulis): no significant alteration of growth rate at 10 ppm +/- 80% increase of growth rate at 50 to 100 ppm (Verschueren 1983).	
Other information	Manufacturing source: petroleum refining. Natural sources (water and air): constituent in paraffin fraction of petroleum (EPA 1975).	

644 • 1-Decanol

112-30-1

Synonyms	Decanol n-Decanol	
Sumformula of the chemical	C10H22O	
Odour	Odour Index at 20 °C: 31000 (Verschueren 1983)	
Molecular weight	158.32	
Specific gravity (water=1)	0.83	at 20/4 °C (Verschueren 1983)
Conversion factor, 1 ppm in air=	6.47	mg/m³ (Verschueren 1983)
Conversion factor, 1 mg/m³ in air=	0.154	ppm (Verschueren 1983)
Vapour pressure, mmHg	1	70 °C
Melting point, °C	-7	
Boiling point, °C	231	
Log octanol/water coefficient, log Pow	4.57	(Sangster 1989)

LD50 values to mammals in oral exposure, mg/kg	4720 6000 12800–25600 6400–12800	orl-rat orl-mus (Lewis & Sweet 1984) orl-rat (n-decyl + sec. decyl) orl-mus (n-decyl + sec. decyl) (Patty 1967)
LD50 values to mammals in non-oral exposure, mg/kg	3560	skn-rbt (Lewis & Sweet 1984)
EC50 values to micro–organims, mg/l	443	Biodegradation inhibition (Vaishnav 1986)
LC50 values to crustaceans, mg/l	4	96hr, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	2.4 7.2	96hr, Pimephales promelas (Veith et al. 1983) 96hr, Alburnus alburnus (Linden et al. 1979)

D

645 • 2-Decanone 693-54-9

Sumformula of the chemical	C10H20O	
Log octanol/water coefficient, log Pow	3.77	(Sangster 1989)
EC50 values to microorganism, mg/l	469	Biodegradation inhibition (Vaishnav 1986)

646 • 1-Decene 872-05-9

State and appearance	Colourless liquid.	
Odour	Threshold Odour Concentration = 0.066 mg/m³ = 11.3 ppb = 0.12 ppm Odour Index at 20 °C = 23 000 000 (Verschueren 1983).	
Specific gravity (water=1)	0.7396	at 20/4 °C (Verschueren 1983)
Vapour pressure, mmHg	1 10 40	at 14.7 °C at 53.7 °C at 83.3 °C (Verschueren 1983)

647 • Dehydroabietic acid 1740-19-8

Synonyms	DHA	
Use	Basis for thermoplastic resins.	
Molecular weight	314.51	
LD50 values to mammals in oral exposure, mg/kg	1710	orl-rat (Lewis & Sweet 1984)

LC50 values to fishes, mg/l	0.77	96hr, Salmo gairdneri (McLeay 1976)
	0.75	96hr, Oncorhynchus kisutch (Anon. 1981)
	0.93	96hr, Oncorhynchus kisutch (Rogers 1975)
	1.38–1.76	96hr, Oncorhynchus kisutch (Davis & Hoos 1975)
	1.1	96hr, Salmo gairdneri (Leach & Thakore 1975)
	1.2	96hr, Salmo gairdneri,
	1.03–1.74	96hr, Salmo gairdneri
	1.38–2.14	96hr, Oncorhynchus nerca (Davis & Hoos 1975)
	1.85	4d, Alburnus alburnus
	1.69	4d, Carassius carassius
	1.01	4d, Coregonus muksun
	0.7	4d, Esox lucius
	1.2	2d, Salmo trutta lacustris (Oikari 1987)
Effects on the physiology of water organisms	Salmo gairdneri; 1.55 mg/l, 4d, change in enzyme activity (Castren & Oikari 1987).	

648 • Dehydroabietol 3772-55-2

LC50 values to fishes, mg/l	0.8	96hr, Salmo gairdneri (Leach & Thakore 1976)

649 • Dehydroacetic acid 520-45-6

Synonyms	3-Aceto-6-methyl-2-pyronone 2H-Pyran-2,4(3H)-dione, 3-acetyl-6-methyl-
Sumformula of the chemical	C8H8O4
EINECS-number	2082939
Water solubility, mg/l	690 (MITI 1992)
Melting point, °C	109–112 (MITI 1992)
Boiling point, °C	270 (MITI 1992)
Total degradation in water	Biodegradation: 84% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

650 • Dehydrojuvabione 16060-78-9

Synonyms	1-Cyclohexene-1-carboxylic acid,4-(1,5-dimethyl-3-oxo-4-hexenyl)-, methyl ester (8CI)	
Molecular formula	C16H24O3	
LC50 values to fishes, mg/l	1.8	96hr, Salmo gairdneri (Leach et al.1975)
	0.8	96hr, Salmo gairdneri (Leach et al.1975) (4'-Dehydrojuvabione)

D

651 • Demephion S-sulfone

2587-94-2

Other information about mammals	ODfr = 75.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

652 • Demeton *

8065-48-3

Synonyms	Systox Demeton-O (CAS 298-03-3) O,O-Diethyl-O-(2-(ethylthio)-ethyl)phosphorothioate Demeton-S (CAS 126-75-0) O,O-Diethyl-S-(2-(ethylthio)-ethyl)-phosphorothioate	
Chemicals in the product	Demeton-O; O,O-diethyl-O-(2-(ethylthio)-ethyl)phosphorothioate; Demeton-S; O,O-diethyl-S-(2-(ethylthio)-ethyl)phosphorothioate	
Use	Systemic insecticide; acaricide.	
State and appearance	Demeton-O is a colourless oil.	
Molecular weight	516.72	
Specific gravity (water=1)	1.12	
Vapour pressure, mmHg	0.00026	20 °C
Water solubility, mg/l	2000	room temperature
Boiling point, °C	123	demeton-O
LD50 values to mammals in oral exposure, mg/kg	1.7 30 1.5	orl-rat (Lewis & Sweet 1984) orl-male-rat (Martin 1968) orl-rat (Martin 1968)
LD50 values to mammals in non-oral exposure, mg/kg	8.2 24	skn-rat skn-rbt (Lewis & Sweet 1984)
LCLo values to mammals in inhalation exposure, mg/kg	15	4hr, ihl-rat (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	7 7.19 2.37–22.0 13.3–39.0 13.3 5.62 1.78 13.3 1.33	orl-bwd orl-dck (Lewis & Sweet 1984) orl-Agelaius phoeniceus orl-Sturnus vulgaris orl-Coturnix coturnix orl-Passer domesticus orl-Quiscalus quiscula orl-Columba livia orl-Quelea quelea 8065-48-3 (Schafer et al. 1983)
Effects on plants	Applications of demeton at 0.56 kg a.i. (24% solution) /ha to about 30 days old tomatoes (Lycopersicon esculentum) as foliar sprays caused a reduction in tomato shoot dry weight (Stephenson et al. 1980).	
LC50 values to crustaceans, mg/l	0.02 0.027	48hr, Daphnia magna (Gorbach & Knauf 1971) 96hr, Gammarus fasciatus (Sanders 1972)

LC50 values to fishes, mg/l	15 1–10	48hr, Cyprinus carpio 24hr Salmo gairdneri (Pesticide Manual 1983)
	> 26.4 5.87 0.055 15.9 0.151	4d, Carassius auratus 4d, Ictalurus punctatus 4d, Lepomis macrochirus 4d, Pimephales promelas 4d, Salmo gairdneri (Holcombe et al. 1987 (systox))
	3.2 0.1	96hr, Pimephales promelas 96hr, Lepomis macrochirus (Pickering et al. 1962)
Other information about water organisms	Aplexa hypnorum, LC50, 4d, > 26.4 mg/l (systox) (Holcombe et al. 1987).	

653 • Demeton-S-methylsulfone 17040-19-6

Synonyms	S-(2-(Ethylsulfonyl)ethyl)-0,0-dimethylphosphorothioate	
Use	Insecticide, acaricide.	
Molecular weight	262.3	
LD50 values to mammals in oral exposure, mg/kg	40 120	orl-rat orl-gpg (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	500	skn-rat (Lewis & Sweet 1984)
LC50 values to crustaceans, mg/l	0.02 0.027	48hr, Daphnia magna (Gorbach & Knauf 1971) 96hr, Gammarus fasciatus (Sanders 1972)
LC50 values to fishes, mg/l	1–10 0.1 15.2	24hr, Salmo gairdneri 96hr, Lepomis macrochirus 48hr, Cyprinus carpio (Sanders 1972)

654 • Desmedipham 13684-56-5

Synonyms	Ethyl m-hydroxycarbanilate carbanilate (ester)
Use	Herbicide.
Effects on plants	1.0 kg desmedipham/ha was applied with a sprayer 24 days after seeding to lamb's-quarters (Chenopodium album L.) in the 3 to 4-leaf stage → decrease in shoot growth and plant number (Jensen et al. 1977).

655 • Dexon 140-56-7

Synonyms	Fenaminosulf	
State and appearance	Yellow brown powder.	
Other physicochemical properties	Decomposes above 200 °C. Solubility 2–3% at 25 °C.	
LD50 values to mammals in oral exposure, mg/kg	64	orl-rat (Anon. 1976)

LD50 values to mammals in non-oral exposure, mg/kg	64	idr-rat (Anon. 1976)
LD50 values to birds in oral exposure, mg/kg	17.8 17.8	orl-Agelaius phoeniceus orl-Sturnus vulgaris (Schafer et al. 1983)
Effects on arthropods	LC50, 24.0 mg/l, 96hr, Pteronarcys californica. (Sanders & Cope 1968)	
LC50 values to crustaceans, mg/l	3.7	96hr, Gammarus lacustris (Sanders 1969)

656 • Di(2-ethylhexyl)adipate 103-23-1

Sumformula of the chemical	C22H4204
EINECS-number	2030901
Water solubility, mg/l	< 10 (MITI 1992)
Melting point, °C	-65 (MITI 1992)
Boiling point, °C	208–218 (4 mmHg) (MITI 1992)
Total degradation in water	Biodegradation: 67–74% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

657 • Di(2-ethylhexyl)fumarate 141-02-6

Synonyms	2-Butenedioic acid (E)-, bis(2-ethylhexyl) ester
Sumformula of the chemical	C20H3604
EINECS-number	2054482
Water solubility, mg/l	< 100 (MITI 1992)
Melting point, °C	< -10 (MITI 1992)
Boiling point, °C	> 300 (MITI 1992)
Total degradation in water	Biodegradation: 73–116% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

658 • Di(2-methoxyethyl)phthalate 117-82-8

Synonyms	DMEP
Use	Plasticizer, especially for cellulose acetate; solvent.
State and appearance	Oily liquid.
Odour	Mild odour.
Boiling point, °C	340
Flashing point, °C	194

Other physicochemical properties	Combustible.

659 • Di-β-naphthol 602-09-5

Other information about mammals	ALD = 42.0 mg/l, act, orl, deer mouse (Virtanen & Nuuja 1987).

660 • Di-2-ethylhexyl sodium salt sulfosuccinate 577-11-7

Sumformula of the chemical	C20H37O7SNa	
Water solubility, mg/l	71000	(MITI 1992)
Total degradation in water	Biodegradation: 0–9% by BOD period: 28d substance: 100 mg/l sludge: 320 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.9 < 9.3	6w, Cyprinus carpio, conc 0.5 mg/l 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
LC50 values to fishes, mg/l	61.3	48hr, Oryzias latipes (MITI 1992)

661 • Di-2-naphthyl disulfide 5586-15-2

Sumformula of the chemical	C20H14S2	
Water solubility, mg/l	< 0.001	(MITI 1992)
Melting point, °C	140	(MITI 1992)
Log octanol/water coefficient, log Pow	> 6.7	(MITI 1992)
Bioconcentration factor, fishes	< 0.3–1.9 < 3.1	6w, Cyprinus carpio, conc 0.2 mg/l 6w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 50	48hr, Oryzias latipes (MITI 1992)

662 • Di-n-amylamine 2050-92-2

State and appearance	Colourless liquid	
Molecular weight	157.29	
Specific gravity (water=1)	0.78	at 20 °C (Verschueren 1983)
Boiling point, °C	202	(Verschueren 1983)
Other information about water organisms	Selmolitus atromaculatus: critical range: 5–20 mg/l, 24hr. (McKee & Wolf 1963)	

663 • 2,6-Di-sec-butylphenol

5510-99-6

Sumformula of the chemical	C14H22O
Water solubility, mg/l	1.8 (MITI 1992)
Melting point, °C	< -10 (MITI 1992)
Boiling point, °C	255–260 (MITI 1992)
Log octanol/water coefficient, log Pow	> 4.30 (MITI 1992)
Total degradation in water	Biodegradation: 3% by GC analysis period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	145–348 8w, Cyprinus carpio, conc 0.0025 mg/l 216–501 8w, Cyprinus carpio, conc 0.00025 mg/l (MITI 1992)
LC50 values to fishes, mg/l	0.47 48hr, Oryzias latipes (MITI 1992)

664 • 2,6-Di-t-butyl-4-ethylphenol

4130-42-1

Sumformula of the chemical	C16H26O
Melting point, °C	43–45 (MITI 1992)
Log octanol/water coefficient, log Pow	> 3.27 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	1420–5060 8w, Cyprinus carpio, conc 0.01 mg/l 930–4870 8w, Cyprinus carpio, conc 0.001 mg/l (MITI 1992)
LC50 values to fishes, mg/l	7.26 48hr, Oryzias latipes (MITI 1992)
Water solubility, mg/l	21 (MITI 1992)

665 • 3,5-Di-tert-butylbiphenyl-4-ol

2668-47-5

Sumformula of the chemical	C20H26O
Water solubility, mg/l	< 10 (MITI 1992)
Melting point, °C	99.8–102.0 (MITI 1992)
Log octanol/water coefficient, log Pow	> 6.19 (MITI 1992)

Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	3380–15900 3260–8690	10w, Cyprinus carpio, conc 0.01 mg/l 10w, Cyprinus carpio, conc 0.001 mg/l (MITI 1992)
LC50 values to fishes, mg/l	460	48hr, Oryzias latipes (MITI 1992)

666 • 2,4-Di-tert-butylphenol 96-76-4

Sumformula of the chemical	C14H22O	
EINECS-number	2025320	
Water solubility, mg/l	35	(MITI 1992)
Melting point, °C	53–57	(MITI 1992)
Log octanol/water coefficient, log Pow	5.19	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	128–436 135–360	8w, Cyprinus carpio, conc 0.02 mg/l 8w, Cyprinus carpio, conc 0.002 mg/l (MITI 1992)
LC50 values to fishes, mg/l	2.67	48hr, Oryzias latipes (MITI 1992)

667 • Diacetone 123-42-2

Synonyms	Diacetone alcohol 4-Hydroxy-4-methyl-2-pentanone Dimethylacetonylcarbinol	
Use	Solvent.	
State and appearance	Colourless liquid, becomes yellow on aging.	
Odour	Quality: sweet Hedonic tone: unpleasant to pleasant Threshold odour concentration absolute: 0.28 ppm 50% recognition: 1.1 ppm 100% recognition: 1.7 ppm Odour index 100% recognition: 776 (Hellman & Small 1974). Odour index at 20 °C = 774. (Verschueren 1983)	
Molecular weight	116.16	
Specific gravity (water=1)	0.93	at 20/4 °C (Verschueren 1983)

Conversion factor, 1 ppm in air=	4.75 mg/m³ (Verschueren 1983)
Conversion factor, 1 mg/m³ in air=	0.216 ppm (Verschueren 1983)
Vapour pressure, mmHg	1 at 20 °C 1.7 at 30 °C
Water solubility, mg/l	> 100000 mg/l (MITI 1992)
Melting point, °C	-57– -43 °C (Verschueren 1983) < -10 (MITI 1992)
Boiling point, °C	169–171 (MITI 1992)
Volatilization	Relative volatility (nBuAc=1) = 0.12
Chemical oxygen demand, g 02/g	2.11 5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.07 5 days (Bridie et al. 1979)
Total degradation in water	Biodegradation: 88–92% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
LD50 values to mammals in oral exposure, mg/kg	4000 orl-rat (Patty 1967)
Other information about mammals	Rat: repeated oral dose; no effect: 0.04 g/kg/day, 30 days inhalation: no deaths: 1500 ppm; 8hr (Patty 1967).
Health effects	Man: irritation of eyes, nose and throat at 100 ppm estimated lethal dose: 30 g (Patty 1967).
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): Pseudomonas putida: 825 mg/l (Bringmann & Kühn 1980a).
LOEC values to algae, mg/l	530 rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1980a)
LC50 values to fishes, mg/l	420 96hr, Lepomis macrochirus 420 96hr, Menidia audens 420 96hr, Menidia beryllina (Dawson et al. 1977) > 5000 24hr, Carassius auratus (Bridie et al. 1979)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): Microcystis aeruginosa 530 mg/l (Bringmann & Kühn 1976) Scenedesmus quadricauda 3000 mg/l (Bringmann & Kühn 1980a) Entosiphon sulcatum 1400 mg/l (Bringmann & Kühn 1980a)

668 • Diallate

2303-16-4

Synonyms	S-2,3-Dichloroallyl-N,N-di-isopropylthiocarbamate
Use	A thiolcarbamate herbicide.
Other information about degradation	Degradation: over 50% loss after 4 weeks incubation in microbiologically active soils with rabid formation of CO2. losses from sterile soils where much slower 30–45% after 20 weeks with only very slow CO2 formation. representative fungi isolated from soils Phoma eupyrena, Penicillium janthinellum and Trichoderma hazzianum could degrade at least 20% of the applied (2.5 ppm) herbicide after 10 days incubation. (Anderson & Domsch 1976)

LD50 values to mammals in oral exposure, mg/kg	395	oral-rat (Anon. 1976)

669 • Diallylamine 124-02-7

Synonyms	Di-2-propenylamine	
Sumformula of the chemical	C6H11N	
Odour	Odour threshold: 8 mg/m³ (Verschueren 1983).	
Molecular weight	97.16	
Specific gravity (water=1)	0.763	at 10/4 °C
Conversion factor, 1 ppm in air=	3.97	mg/m³ (Verschueren 1983)
Conversion factor, 1 mg/m³ in air=	0.252	ppm (Verschueren 1983)
Water solubility, mg/l	86000	
Melting point, °C	-88.4	
Boiling point, °C	111–112	(Verschueren 1983)
pKa	9.29	(Sangster 1989)
Log octanol/water coefficient, log Pow	1.11	(Sangster 1989)
Chemical oxygen demand, g 02/g	2.5	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.06	5 days (Bridie et al. 1979)
Other information about degradation	Degradation by Aerobacter: 200 mg/l at 30 °C: parent: 62% degradation in 105hr mutant: 100% degradation in 17hr (Verschueren 1983)	
LD50 values to mammals in oral exposure, mg/kg	578	oral-rat (Patty 1967)
LC50 values to mammals in inhalation exposure, mg/m³	2755 795	4hr, ihl-rat Patty 1967 8hr, ihl-rat (Patty 1967)
Other information about mammals	Rat: inhalation: deaths: 200 ppm, 50 x 7hr inhalation: change in liver and kidneys: 20 ppm, 50 x 7hr (Patty 1967)	
LC50 values to fishes, mg/l	20	96hr, Carassius auratus (Bridie et al. 1979)

670 • Diallylpthalate 131-17-9

State and appearance	Nearly colourless oily liquid.	
Specific gravity (water=1)	1.12	at 20/20 °C (Verschueren 1983)
Water solubility, mg/l	46	(MITI 1992)
Melting point, °C	-70 < -10 (MITI 1992)	
Boiling point, °C	160	at 4 mm (Verschueren 1983)

Total degradation in water	Biodegradation: 76–92% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): Pseudomonas putida: > 100 mg/l (Bringmann & Kühn 1980a).
LOEC values to algae, mg/l	0.65 rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976) 2.9 rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): Microcystis aeruginosa 0.65 mg/l (Bringmann & Kühn 1976) Scenedesmus quadricauda 2.9 mg/l (Bringmann & Kühn 1980a) Entosiphon sulcatum 13 mg/l (Bringmann & Kühn 1980a) Uronema parduczi Chatton-Lwoff 22 mg/l (Bringmann & Kühn 1980b)

671 • Diamidafos 1754-58-1

Synonyms	Nellite
Hydrolysis in water	At pH 7.1 and 7.9, no detectable chemical hydrolysis took place within a period of 22 days (Meikle 1978).
Hydrolysis in acid	Acid hydrolysis yielded N-methyl-hydrogen phosphoro-amidate and dihydrogen phenylphosphate (Meikle 1978).
Hydrolysis in base	At pH 4.1 the chemical hydrolysis rate was such that at 25 °C the half-life was 39.8 days (Meikle 1978).
LD50 values to birds in oral exposure, mg/kg	13.3 orl-Agelaius phoeniceus 75 orl-Sturnus vulgaris (Schafer et al. 1983)

672 • 1,3-Diamino-2-propanol tetraacetic acid 3148-72-9

Use	Chelating agent.
Molecular weight	322
Effects on wastewater treatment	Impact on conventional biologial treatment systems: *chemical conc. mg/l* — *effect* unacclimated system 1000 inhibitory acclimated system 584 biodegradable Only slight inhibition was exhibited by the unacclimated biomass. The compound, at the concentration tested, was amenable to moderate biodegradation (Anon. 1974).
LC50 values to crustaceans, mg/l	> 100 Daphnia magna (Anon. 1974)
LC50 values to fishes, mg/l	> 300 Pimephales promelas (Anon. 1974)
Other information about water organisms	Selenastrum capricornutum: 1 mg/l, no effect 10 mg/l, inhibitory 100 mg/l, inhibitory (Anon. 1974).

673 • 1,2-Diaminobenzene 95-54-5

Synonyms	o-Phenylenediamine
LD50 values to birds in oral exposure, mg/kg	133 orl-Agelaius phoeniceus > 1000 orl-Sturnus vulgaris > 1000 orl-Coturnix coturnix 100 orl-Passer domesticus (Schafer et al. 1983)
Other information about water organisms	EC50 (60hr), 48 mg/l, rpd, Tetrahymena pyriformis (Schulz & Applehans 1985).

674 • 1,3-Diaminobenzene 108-45-2

Synonyms	1,3-Benzenediamine m-Phenylenediamide
State and appearance	Colourless needles.
Molecular weight	108.16
Water solubility, mg/l	351 900 (MITI 1992)
Melting point, °C	63–64
Boiling point, °C	282–284 (MITI 1992)
Log octanol/water coefficient, log Pow	-0.38 (MITI 1992)
Total degradation in soil	Biodegradation: decomposition by soil microflora in > 64 days (Verschueren 1983).
Total degradation in water	Biodegradation: 2% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	1.3–4.6 6w, Cyprinus carpio, conc 2 mg/l < 1.6–24 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	650 orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	90 unk-mus (Lewis & Sweet 1984)
LDLo values to mammals in oral exposure, mg/kg	300 orl-cat, orl-rbt (Lewis & Sweet 1984)
LDLo values to mammals in non-oral exposure, mg/kg	5000 skn-rbt (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	> 1000 orl-Agelaius phoeniceus > 1000 orl-Sturnus vulgaris 562 orl-Coturnix coturnix > 1000 orl-Passer domesticus (Schafer et al. 1983)
LC50 values to fishes, mg/l	5.74 48hr, Carassius auratus (McKee & Wolf 1963) > 500 48hr, Oryzias latipes (MITI 1992)

675 • 1,4-Diaminobenzene 106-50-3

Synonyms	p-Phenylenediamine	
LD50 values to birds in oral exposure, mg/kg	100	orl-Agelaius phoeniceus
	562	orl-Sturnus vulgaris
	100	orl-Coturnix coturnix
	422	orl-Passer domesticus (Schafer et al. 1983)
Other information about water organisms	EC50 (60hr), 74 mg/l, rpd, Tetrahymena pyriformis (Schulz & Applehans 1985).	

676 • 1,5-Diaminonaphthalene 2243-62-1

Water solubility, mg/l	380	(MITI 1992)
Melting point, °C	185–187	(MITI 1992)
Log octanol/water coefficient, log Pow	0.91	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.4–1.5	6w, Cyprinus carpio, conc 0.2 mg/l
	< 4.5	6w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
LC50 values to fishes, mg/l	31.5	48hr, Oryzias latipes (MITI 1992)
Other information about water organisms	EC50 (60hr), 45 mg/l, rpd, Tetrahymena pyriformis (Schulz & Applehans 1985).	

677 • 1,8-Diaminonaphthalene 479-27-6

Water solubility, mg/l	850	(MITI 1992)
Melting point, °C	61–62	(MITI 1992)
Log octanol/water coefficient, log Pow	2.21	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	3.6–6.1	6w, Cyprinus carpio, conc 0.1 mg/l
	< 3.7–6.5	6w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
LC50 values to fishes, mg/l	12.3	48hr, Oryzias latipes (MITI 1992)
Other information about water organisms	EC50 (60hr), 23 mg/l, rpd, Tetrahymena pyriformis (Schulz & Applehans 1985).	

678 • 2,3-Diaminonaphthalene

771-97-1

Other information about water organisms	EC50 (60hr), 55 mg/l, rpd, Tetrahymena pyriformis (Schulz & Applehans 1985).

679 • 2,4-Diaminophenol hydrochloride

137-09-7

Synonyms	Amidol
State and appearance	Grayish white crystals.
Other information about water organisms	Goldfish: approx. fatal conc. 80 mg/l, 48hr (McKee & Wolf 1963).

680 • 2,4-Diaminotoluene

95-80-7

Synonyms	4-Methylphenylene-1,3-diamine	
Melting point, °C	99	(MITI 1992)
Boiling point, °C	280	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).	
Bioconcentration factor, fishes	< 5 < 50	6w, Cyprinus carpio, conc 0.3 mg/l 6w, Cyprinus carpio, conc 0.03 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	850	48hr, Oryzias latipes (MITI 1992)

681 • o-Dianisidine

119-90-4

Synonyms	Di-p-amino-di-m-methoxydiphenyl 3,3'-Dimethoxybenzidine
State and appearance	Colourless crystals.
Melting point, °C	137
Other information about degradation	Biodegradation rates: degradation by Aerobacter: 500 mg/l at 30 °C % ring disruption: parent: 78% in 120hr mutant: 100% in 36hr (Verschueren 1983).

682 • Diazinon

333-41-5

Synonyms	O,O-Diethyl-O-(2-isopropyl-6-methyl-pyrimidin-4-yl-phosphorothioate) O,O-Diethyl-O-(2-propyl-6-methylpyrimidin-4-yl)-thiophosphate O,O-Diethyl-O-(2-isopropyl-4-methyl-6-pyrimidinyl)thiophosphoric acid
Sumformula of the chemical	C12H21N2O3PS

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Known impurities	Sulfotepp: 1.4–6.9 ppm as impurity. (Meier et al. 1979)	
Use	Active ingredient in insecticides.	
State and appearance	a colourless oil (decomposes above 120 °C)	
Molecular weight	304.38	
Specific gravity (water=1)	1.116	
Vapour pressure, mmHg	1.29	at 20 °C (KEMI 1991)
Water solubility, mg/l	40	20 °C
Boiling point, °C	83–84	(MITI 1992)
pKa	2.39	(KEMI 1991)
Log octanol/water coefficient, log Pow	3.95	(KEMI 1991)
Log soil sorption coefficient, log Kom	2.12	(Sabljic 1987)
Mobility	The mobility of diazinon is medium high. It is bound more tightly to soil the higher is contents of humus in soil, the dryer soil is and the lower temperature is in soil. Ka: 2–325, Koc: 255–496 (KEMI 1991). Decomposes above 120 °C.	
Hydrolysis in water	Diazinon is transformed nearest by hydrolysis. The transformation is relative slow. It depends on acidity in soil or water; the sourer soil the quicklier transformation (KEMI 1991).	
Hydrolysis in acid	Acid hydrolysis (pH ü 2) reduced diazinon concentration by > 99.9%; hydrolysis products are 6-isopropyl-4-methyl-2-pyrimidinol and thiophosphate (Meier et al. 1976).	
Half-life in soil, days	32	(Li et al. 1990)
Total degradation in soil	75–100% disappearance from soils: 12 weeks (Verschueren 1983). Persistence in soil at 10 ppm initial concentration: *wk incubation to* *50% remaining* / *5% remaining* sterile sandy loam: 12.5 / - sterile organic soil: 6.5 / - non-sterile sandy loam: < 1 / 1 non-sterile organic soil: 2 / 7 (Miles et al. 1979)	
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Other information about degradation	In soil diazinon is degraded by microorganisms under acidic conditions. It is happening more quicklier if the soil is misty and it has low pH and high temperature. In the laboratory experiment half of diazinon was mineralized after five months at 25 °C. Degradation of diazinon by microbies is happening also in water. The half-life in water is about 3 days in the laboratory experiment. (KEMI 1991) In the degradation (clay soil) pyrimidinol and hydroxypyrimidinol are the degradation products. Pyrimidinol degradates in acidic conditions to carbon dioxide. Diazinon transforms even to diazoxon and hydroxydiazinon. Diaoxon is more toxicity than diazinon. (KEMI 1991)	

Bioconcentration factor, fishes	96.7–210 Pseudorasbora parva (Verschueren 1983) 10 Fundulus heteroclitus (Verschueren 1983) 0–46.9 6w, Cyprinus carpio, conc 0.04 mg/l 10.7–36.6 6w, Cyprinus carpio, conc 0.004 mg/l (MITI 1992)
Bioconcentration factor, other organisms	4.9–152 water organisms (Verschueren 1983)
Other information about bioaccumulation	Bioconcentration ratios of diazinon by various species of freshwater organisms – exposed to 10 ppb for 7 days: *bioconcentration ratio average* Pseudorasbora parva 152 Cyprinus auratus 36.6 Cyprinus carpio 65.1 Lebistes reticulatus 17.5 Procambarus clarkii 4.9 Indoplanorbis exustus 17.0 Cipangopoludina malleata 5.9 Pseudorasbora parva: bioconcetration ratio increased with body weight (exposure at 10 ppb for 7 days) from 50 to 175 for body weights between 2 and 6 g. (Kanazawa 1978) Effect of the diazinon concentration in test water on the bioconcentration ratios by Pseudorasbora parva: *diazinon in water, ppb* / *days after exposure* / *bioconc. ratio* / *days after return to clean water* / *diazinon in fish, ppb* 11.5 / 7 / 118.2 / 8 / 5 52.5 / 7 / 206.0 / 7 / 26 (Kanazawa 1978) Diazinon is moderately bioaccumulated. log Kow: 3.95; BCF in fish 18–213. (KEMI 1991) Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	300–400 oral-rat, techn.grade (Anon. 1976) 423–1031 orl-rat (KEMI 1991)
LD50 values to mammals in non-oral exposure, mg/kg	455 skn-rat 400 skn-rbt (Lewis & Sweet 1984) 900 skn-rat-male (Martin 1968) 455 skn-rat-female (Martin 1968) > 2150 skn-rat (KEMI 1991)
LC50 values to mammals in inhalation exposure, mg/m³	3500 ihl-rat (KEMI 1991)
LDLo values to mammals in oral exposure, mg/kg	30 orl-rbt (Lewis & Sweet 1984)

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LD50 values to birds in oral exposure, mg/kg	2	orl-bwd
	3.5	orl-dck (Lewis & Sweet 1984)
	00–3.16	orl-Agelaius phoeniceus
	110–316	orl-Sturnus vulgaris
	4.22	orl-Coturnix coturnix
	7.5	orl-Passer domesticus
	7.5	orl-Quiscalus quiscula
	3.16	orl-Columba livia (Schafer et al. 1983)
	1–10	quail, sparrow, duck (KEMI 1991)
Subacute LC50 values to birds in feeding exposure, mg/kg	32–38	5d, mg/kg, feed, Anas platyrhynchos (KEMI 1991)
Effects on reptiles	Diazinon (12 mg/kg soil) hinders the growth of young earthworms (Allolobophora calignosa) (KEMI 1991).	
Effects on bees	Highly toxic to bees (Martin 1968). LD50, 48hr, 0.37 µg/bee (KEMI 1991).	
Effects on arthropods	LC50, 0.025 mg/l, 96hr, Pteronarcys californica (Sanders & Cope 1968) LC50, 0.0046 mg/l, 30d, Pteronarcys dorsata NOEC, 0.0039 mg/l, 30d, Pteronarcys dorsata (Verschueren 1983) LC50, 0.0017 mg/l, 96hr, Acroneuria lycorias LC50, 0.00125 mg/l, 30d, Acroneuria lycorias NOEC, 0.00083 mg/l, 30d, Acroneuria lycorias LC50, 0.0022 mg/l, 30d, Ophiogomphus rubinsulensis NOEC, 0.00129 mg/l, 30d, Ophiogomphus rubinsulensis LC50, 0.00354 mg/l, 30d, Hydropsyche bettoni NOEC, 0.00179 mg/l, 30d, Hydropsyche bettoni LC50, 0.00105 mg/l, 30d, Ephemerelia subvaria NOEC, 0.00042 mg/l, 30d, Ephemerelia subvaria LD50, 2450 ppm, rice field spider: Oedothorax insecticeps (Ishikura 1972) LC50, misty soil, 1.2 mg/kg soil, grasshopper LC50, dry soil, 37.6 mg/kg soil, grasshopper (KEMI 1991)	
Effects on plants	Application of diazonin at 0.42 kg a.i. (50% emulsifiable concentrate)/ha to about 30 days old tomatoes (Lycopersicon esculentum) as foliar sprays caused a reduction in tomato shoot dry weight (Stephenson et al. 1980).	
EC50 values to algae, mg/l	6.4	grw, 7d, Selenastrum capricornitum
	17.3	grw, 5d, Scenedesmus subspicatus (KEMI 1991)
NOEC values to algae, mg/l	0.06	7d, Selenastrum capricornitum (KEMI 1991)
LC50 values to crustaceans, mg/l	0.00027	30d, Gammarus pseudolimnesus (Verschueren 1983)
	0.0026	96hr, Acartia tonsa (Khattat & Farley 1976)
	0.0012	48hr, Daphnia magna (Dennis et al. 1979)
	2.27	96hr, Saccobranchus fossilis (Verma et al. 1982)
	0.08	Daphnia pulex (Hashimoto & Nishiuchi 1981)
	0.008	D.pulex (Nishiuchi & Hashimoto 1967)
	0.004	act, Daphnia magna (Kenaga 1979)
	0.0009	48hr, Daphnia pulex (Sanders & Cope 1966)
	0.0025	48hr, Daphnia magna (Gorbach & Knauf 1971)
	0.2	96hr, Gammarus lacustris (Sanders 1969)
	0.0014	48hr, Simocephalus serrulatus (Sanders & Cope 1966)

EC50 values to crustaceans, mg/l	0.0009 48hr, Daphnia pulex (Shapiro 1979) 0.00096–0.0011 48hr, mg/l, Daphnia magna (KEMI 1991)
LOEC values to crustaceans, mg/l	0.00032 mbt, Daphnia magna (KEMI 1991)
NOEC values to crustaceans, mg/l	0.00024 rpd, 21d, Daphnia magna (Biesinger 1973) 0.0002 30d, Gammarus pseudolimneaus 0.00026 21d, Daphnia magna (Verschueren 1983) 0.00056 48hr, Daphnia magna (KEMI 1991) 0.00083 chronic, rpd, Daphnia magna (KEMI 1991)
LC50 values to fishes, mg/l	0.09 act, Salmo gairdneri (Kenaga 1979) 0.052 24hr, Lepomis macrochirus 0.38 24hr, Salmo gairdneri (Cope 1965) 7.8 96hr, Pimephales promelas 1.6 96hr, Jordanella floridae 0.77 96hr, Salvelinus fontinalis 0.46 96hr, Lepomis macrochirus 0.45 96hr, Salmo trutta m. lacustris (Allison & Hermanutz 1977) 1.9 24hr, Cyprinus carpio (Hashimoto et al. 1982) 3.1 96hr, Channa punctata (Sastry & Malik 1981) 3.2 48hr, Cyprinus carpio 5.1 48hr, Carassius auratus (Hashimoto & Nishiuchi 1981) 2.6–3.2 96hr, Salmo gairdneri 16 96hr, Lepomis macrochirus 7.6–23.5 96hr, Cyprinus carpio (Pesticide Manual 1983) 3.2 48hr, Cyprinus carpio (Nishiuchi & Hashimoto 1967) 0.02 Lepomis macrochirus (Kenaga 1979) 2.3 1d, Branchydanio rerio, 2.12 4d, Branchydanio rerio, (Ansari et al. 1987) 0.45–1.05 96hr, Salvelinus fontanalis (Allison & Hermanutz 1977) 3.7–10.0 96hr, Pimephales promelas 0.17–0.53 96hr, Lepomis macrochirus (Dennis et al. 1979) 0.4 96hr, Salmo gairdneri (KEMI 1991) 23 96hr, Cyprinus carpio (KEMI 1991) 4 48hr, Oryzias latipes (MITI 1992)
LOEC values to fishes, mg/l	0.014 grw, chr, Platichthys flesus (Allison & Hermanutz 1977) 0.09 rpd, schr, Pimephales promelas (Järvinen & Tanner 1982) 0.0005 rdp, schr, Cyprinodon variegatus (Goodman et al. 1979) 0.0032 chr, Pimephales promelas (Allison & Hermanutz 1977)
NOEC values to fishes, mg/l	0.04 rpd, schr, Pimephales promelas (Järvinen & Tanner 1982) 0.008 chr, Pimephales promelas (Allison & Hermanutz 1977)
Other information	Decomposes above 120 °C.

683 • Dibenz(a, h)anthracene 53-70-3

Synonyms	1,2:5,6-Dibenzanthracene
Sumformula of the chemical	C22H14
Log octanol/water coefficient, log Pow	6.75 (Sangster 1989)
Log soil sorption coefficient, log Kom	6.31 observed (Sabljic 1987) 6.44 calculated (Sabljic 1987)
Other information about water organisms	Lethal threshold concentration (LT50): 0.0004 mg/l, 0.13 d (Newsted & Giesy 1987).

684 • Dibenzofuran 132-64-9

Synonyms	Diphenylene oxide
Sumformula of the chemical	C12H8O
Water solubility, mg/l	< 10 (MITI 1992)
Melting point, °C	86 (MITI 1992)
Boiling point, °C	287 (MITI 1992)
Log octanol/water coefficient, log Pow	4.12 (Mackay 1982) 4.12 (Sangster 1989) 5.16 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	524–2420 8w, Cyprinus carpio, conc 0.05 mg/l 848–2200 8w, Cyprinus carpio, conc 0.005 (MITI 1992)
Other information about bioaccumulation	Confirmed to be accumulated on a medium level (Anon. 1987).
LD50 values to birds in oral exposure, mg/kg	> 102 orl-Agelaius phoeniceus (Schafer et al. 1983)
LC50 values to fishes, mg/l	1.78–1.85 96hr, Pimephales promelas (Geiger et al. 1988) 4.2 48hr, Oryzias latipes (MITI 1992)

685 • 2,2'-Dibenzothiazolyl disulfide 120-78-5

Synonyms	Benzothiazole, 2,2'-dithiobis-
Sumformula of the chemical	C14H8N2S4
EINECS-number	2044249
Water solubility, mg/l	< 10 (MITI 1992)
Melting point, °C	178 (MITI 1992)

Total degradation in water	Biodegradation: 0.8% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	1.0–7.2 < 1.4–51	6w, Cyprinus carpio, conc 0.2 mg/l 6w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
LC50 values to fishes, mg/l	19	48hr, Oryzias latipes (MITI 1992)

686 • Dibenzothiophene

132-65-0

Sumformula of the chemical	C12H8S	
Use	Cosmetics and pharmaceuticals, intermediate.	
State and appearance	Colourless crystals.	
Water solubility, mg/l	0.7	(MITI 1992)
Melting point, °C	97–100	(MITI 1992)
Boiling point, °C	332–333 (MITI 1992)	
Log octanol/water coefficient, log Pow	4.38 4.42	(Sangster 1989) (MITI 1992)
Log soil sorption coefficient, log Kom	4.05 4	observed (Sabljic 1987) calculated (Sabljic 1987)
Total degradation in water	Biodegradation: 0–1% by BOD period: 28d substance: 100 mg/l sludge: 30mg/l (MITI 1992).	
Bioconcentration factor, fishes	1220–2410 817–1440	8w, Cyprinus carpio, conc 0.1 mg/l 8w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
LC50 values to fishes, mg/l	106	48hr, Oryzias latipes (MITI 1992)

687 • Dibenzoyl peroxide

94-36-0

Synonyms	Benzoylperoxide	
Water solubility, mg/l	9.1	(MITI 1992)
Total degradation in water	Biodegradation: 84% by BOD period: 21d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	

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688 • Dibenzyl toluene 26898-17-9

Water solubility, mg/l	< 0.1 (MITI 1992)
Boiling point, °C	390 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	397–2410 10w, Cyprinus carpio, conc 0.001 mg/l 785–6160 10w, Cyprinus carpio, conc 0.001 mg/l 301–2400 10w, Cyprinus carpio, conc 0.001 mg/l 349–4020 10w, Cyprinus carpio, conc 0.001 mg/l 552–2860 10w, Cyprinus carpio, conc 0.0001 mg/l 1180–8180 10w, Cyprinus carpio, conc 0.0001 mg/l 807–3400 10w, Cyprinus carpio, conc 0.0001 mg/l 590–6190 10w, Cyprinus carpio, conc 0.0001 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be accumulated on a medium level (Anon. 1987).
LC50 values to fishes, mg/l	505 48hr, Oryzias latipes (MITI 1992)

689 • Dibenzylether 103-50-4

Water solubility, mg/l	< 10 (MITI 1992)
Boiling point, °C	295–298 (MITI 1992)
Log octanol/water coefficient, log Pow	3.4 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	171–429 8w, Cyprinus carpio, conc 0.2 mg/l 187–345 8w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	18 48hr, Oryzias latipes (MITI 1992)

690 • 1,3-Dibromo-2,2-bis(bromo-methyl)propane 3229-00-3

Water solubility, mg/l	1.6 (MITI 1992)
Melting point, °C	157.5–158.5 (MITI 1992)
Log octanol/water coefficient, log Pow	3.99 (MITI 1992)

Total degradation in water	Biodegradation: 29% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	7.1–102 8w, Cyprinus carpio, conc 2 mg/l 289–548 8w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	> 200 48hr, Oryzias latipes (MITI 1992)

691 • 1,2-Dibromo-3-chloropropane 96-12-8

Synonyms	3-Chloro-1,2-dibromopropane DBCP
Use	Soil fumigant; nematocide; intermediate in organic synthesis; LW grade (low in volatiles) commercial preparations of the flame retardant tris((2,3-dibromopropyl)phosphate) contained DBCP in the order of 0.05%.
State and appearance	Amber to dark brown liquid.
Odour	Mildly pungent odour.
Specific gravity (water=1)	2.08 at 20/20 °C (Verschueren 1983)
Vapour pressure, mmHg	0.8 at 21 °C (Verschueren 1983)
Water solubility, mg/l	1000 at room temp. (Verschueren 1983) 300 (MITI 1992)
Boiling point, °C	196 (MITI 1992)
Log octanol/water coefficient, log Pow	2.96 (MITI 1992)
Total degradation in soil	Persistence: fields treated with DBCP contained still 2 to 5 ppb in the topsoil after 2 to 4 years (Peoples et al. 1980).
Other information about degradation	Aquatic reactions: DBCP is converted by soil water cultures to n-propanol. The maximum conversion rate observed (Br-/2DBCP0) is 63% in the course of 4 weeks-initial conc. 0.001 M DBCP: $CH_2BrCHBrCH_2Cl \xrightarrow[pH\ 7.5]{soil\text{-}H_2O} CH_3CH_2CH_2OH + 2Br^- + Cl^-$ (Castro & Belsen 1968).
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon.1987).
LD50 values to mammals in oral exposure, mg/kg	173 orl-rat (Martin 1968) 257 orl-male-mus (Martin 1968) 270–620 orl-female-mus (Martin 1968)
LD50 values to mammals in non-oral exposure, mg/kg	1420 skn-rbt (Martin 1968)
Other information about mammals	In diet: in 90 day feeding tests with rats, the lowest level causing a decrease in growth rate was 150 ppm for females and 450 ppm for males. (Martin 1968)
Health effects	Man: occurrence of primary disruption of spermatogenesis at the testicular level for all users who had extensive exposure to the compound-among them formulators, custom applicators, and farmers. (Sandifer et al. 1979)

Bioconcentration factor, fishes	3.6–17 6w, Cyprinus carpio, conc 0.3 mg/l 4.0–19 6w, Cyprinus carpio, conc 0.03 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	35 48hr, Oryzias latipes (MITI 1992)

692 • p-Dibromobenzene 106-37-6

Sumformula of the chemical	C6H4Br2
EINECS-number	2033902
Water solubility, mg/l	< 0.01 (MITI 1992)
Melting point, °C	86.9 (MITI 1992)
Boiling point, °C	218–219 (MITI 1992)
Log octanol/water coefficient, log Pow	3.58 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	42.9–313 8w, Cyprinus carpio, conc 0.01 mg/l 44.2–279 8w, Cyprinus carpio, conc 0.001 mg/l (MITI 1992)
LC50 values to fishes, mg/l	32.8 48hr, Oryzias latipes (MITI 1992)

693 • 4,4'-Dibromobiphenyl 92-86-4

Sumformula of the chemical	C12H8Br2
EINECS-number	2021986
Water solubility, mg/l	< 10 (MITI 1992)
Melting point, °C	166–168 (MITI 1992)
Log octanol/water coefficient, log Pow	6.68 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	8100–19900 8w, Cyprinus carpio, conc 0.01 mg/l 1300–6170 8w, Cyprinus carpio, conc 0.001 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 100 48hr, Oryzias latipes (MITI 1992)

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694 • Dibromocresyl glycidyl ether 30171-80-3

Melting point, °C	5–10 (MITI 1992)
Boiling point, °C	172 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 1.3 6w, Cyprinus carpio, conc 0.03 mg/l < 13 6wCyprinus carpio, conc 0.003 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	3.6 48hr, Oryzias latipes (MITI 1992)

695 • 1,10-Dibromodecane 4101-68-2

Water solubility, mg/l	< 10 mg/l (MITI 1992)
Melting point, °C	28 (MITI 1992)
Boiling point, °C	127–130 (MITI 1992)
Log octanol/water coefficient, log Pow	6.12 (MITI 1992)
Total degradation in water	Biodegradation: 14–18% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	103–320 8w, Cyprinus carpio, conc 50 000 mg/l 12–108 8w, Cyprinus carpio, conc 5 000 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	8.33 48hr, Oryzias latipes (MITI 1992)

696 • Dibromoneopentylglycol 3296-90-0

Sumformula of the chemical	C5H10O2Br2
Water solubility, mg/l	38000 (MITI 1992)
Melting point, °C	111–113 (MITI 1992)
Log octanol/water coefficient, log Pow	2.29 (MITI 1992)
Total degradation in water	Biodegradation: 3–33% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

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Bioconcentration factor, fishes	0.8–1.1 < 4.8	6w, Cyprinus carpio, conc 3 mg/l 6w, Cyprinus carpio, conc 3 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 500	48hr, Oryzias latipes (MITI 1992)

697 • 2,3-Dibromosuccinic acid 526-78-3

Water solubility, mg/l	> 1000	(MITI 1992)
Melting point, °C	266	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.3 < 3.0–10	6w, Cyprinus carpio, conc 0.2 mg/l 6w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	235	48hr, Oryzias latipes (MITI 1992)

698 • Dibutyl phthalate 84-74-2

Synonyms	Di-n-butylphthalate Phthalic acid, dibutyl ester 1,2-Benzenedicarboxylic acid, dibutylester	
Sumformula of the chemical	$C_{16}H_{22}O_4$	
Purity, %	100	
Use	Plasticizer manufacturing; plastics manufacturing; recycling and processing. Insect repellent for the impregnation of clothing. Explosives.	
State and appearance	Colourless oily liquid will sink and associate with sediments. Very little will dissolve.	
Odour	Mild odour.	
Molecular weight	278.38	
Specific gravity (water=1)	1.048	
Vapour density (air=1)	9.58	
Vapour pressure, mmHg	0.1 < 10 200	115 °C 25 °C 287 °C
Water solubility, mg/l	28–4000 10.1	25–26 °C 20 °C
Melting point, °C	-35	
Boiling point, °C	340	1013 hPa
Flashing point, °C	157	
Log octanol/water coefficient, log Pow	4.79 4.6–4.9	(Anon. 1988) (Anon. 1989)

Henry's law constant, Pa x m³/mol	0.12 (Anon. 1988) 0.27 25 °C (Anon. 1989)
Adsorption/desorption	Phthalate esters are readily sequestered by or absorbed on organic residues and solid surfaces in environmental water systems. Accumulation and subsequent long-term low-level release are theorized (Sax 1986).
Mobility	Equilibrium distribution: *mass %* air 0.38 water 9.52 solid 90.1 (Anon. 1988). Theoretical distribution: > 90% in sediment and soil, approximately 8% in water (Nordic 1988). Flammability: slight when exposed to heat or flame. Toxic combustion products: slight hazard. Practically insoluble in water (Sax 1986).
Hydrolysis in water	Hydrolysis very slow (Giam et al. 1984).
Half-life in soil, days	180 > 6 months (Shea et al. 1982)
Aerobic degradation in soil	Aerobic degradation in freshwater hydrosoil: 98% alter 5 days incubation (Verschueren 1983)
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
Other information about degradation	Degradation of di-butyl-phthalate:

ENVIRONMENT	*INIT.CONC. mg/l*	*REDOX-COND.*	*TEMP. °C*	*DEGRADATION %/day*	*REF.*
water	5	aerobic	25	100/7	a
water	10	aerobic	25	100/7	a
freshwater sediment	1	aerobic	22	5/1	b
freshwater sediment	1	aerobic	22	95/7	b
freshwater sediment	1	aerobic	22	97/30	b
freshwater sediment	1	anaerobic	22	0/1	b
freshwater sediment	1	anaerobic	22	47/7	b
freshwater sediment	1	anaerobic	22	98/30	b
sludge	100	aerobic	30	> 90/20	c
soil	0.00045	aerobic	20	0/14	d
soil (adapted)	0.00045	aerobic	20	75/14	d
soil	500	aerobic	30	100/15	e
soil	500	anaerobic	30	60/30	e
soil	1000	aerobic	4	2/53	f
soil	1000	aerobic	23	32/53	f
soil	1000	aerobic	23	88/200	f
soil	1000	aerobic	30	78/53	f
soil	1000	anaerobic	23	69/53	f
soil	1000	anaerobic	23	98/200	f
soil	1.4	aerobic	25	100/1	g
soil (sterile)	1.8	aerobic	25	70/5	g
soil	1.4	aerobic	25	100/2	g
soil (sterile)	1.1	aerobic	25	72/5	g
soil	5.1	aerobic	10	t1/2= 5.6	h

a) Tabak et al. 1981
b) Johnson & Luives 1975
c) Engelhardt et al. 1977
d) Hutchins & Ward 1984
e) Shanker et al. 1985
f) Inman et al. 1984
g) Russell et al. 1985
h) Lökke 1984
(Anon. 1987b).

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	Easily biodegradable both in aerobic and anaerobic ways (Kaare Jensen et al. 1987). Easily degradable (Anon. 1989). In sediment and soil relatively slow degradation (Giam et al. 1984). Degradation products of special interest: monobutyl phthalate, assumed toxic metabolite in Artemia (Hudson et al. 1981).
Other information about metabolism	Food chain contamination potential: ester is taken up rapidly and magnified in crustacea, but clears after 10 days. Negative (Sax 1986).
Bioconcentration factor, fishes	12 24hr, Cyprinodon (Wofford et al. 1981)
Bioconcentration factor, crustaceans	5000 Palaemonetes kadiakensis (Verschueren 1983) 140 10d, Gammarus pulex (Thuren & Woin 1988) 1400 14d, Gammarus pseudolimnaeus, total (Mayer & Sanders 1973) 5000 7d, Daphnia 6500 7d, Gammarus pseudolimnaeus (Sanders et al. 1973)
Bioconcentration factor, other organisms	6600 7d, Chironomus (Sanders et al. 1973)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987). After 24hr exposure of fish only 13% appears as dibutyl phthalate and 48% as flatic acid (Wofford et al. 1981). Often higher concentrations in sediment (0.00016 mg/g) as in animals living in sediment (0.00010 mg/g) (Ray et al. 1983).
LD50 values to mammals in oral exposure, mg/kg	8000 orl-rat (Lewis & Sweet 1984) 1000 orl-rbt 12000 orl-rat 5.282 orl-mus (Sax 1986)
LD50 values to mammals in non-oral exposure, mg/kg	3050 ipr-rat 3570 ipr-mus 720 ivn-mus (Sax 1986)
LC50 values to mammals in inhalation exposure, mg/m³	7.9 ihl-rat (Lewis & Sweet 1984) 2.1 ihl-mus 9620 ihl-mam (Sax 1986)
TDLo values to mammals in oral exposure, mg/kg	8.4 orl-rat, 7d male, teratogenic effect 2520 orl-rat, 1-21d preg, teratogenic eff. 12600 orl-rat, 1-21d preg, teratogenic eff. 1440 orl-mus, 1-18d preg, teratogenic eff. 12000 orl-mus, 1-18d preg, teratogenic eff. 38000 orl-mus, 1-18d preg, teratogenic eff. 16800 orl-mus, 7d male, teratogenic effect 14000 orl-gpg, 7d male, teratogenic effect (Sax 1986) 140 orl-hmn (Sax 1986)
TDLo values to mammals in non-oral exposure, mg/kg	1017 ipr-rat, 5-15d preg, teratogenic effect 305 ipr-rat, 5-15d preg, teratogenic effect 6000 ipr-rat, 3-9d preg, teratogenic effect (Sax 1986)

Effects on the physiology of mammals	Induces many biochemical effects, e.g. increases liver cytochrome P-450, reduces serum albumine, changes active K-ion transportation via membranes (Giam et al. 1984).	
Health effects	Man, oral, lowest dose which affects the central nervous system: 140 mg/kg (Sax 1986). Direct contact; low, eye, skin (Sax 1986).	
Mutagenicity	Negative in Drosophila-test. No x-chromosome mutations noted in male fluit flies fed sublethal doses (Sax 1986). cyt, ham, fbr, 30 mg/l, 24hr (Sax 1986).	
Teratogenicity	Positive. Teratogenic effects demonstrated in rats (Sax 1986).	
Effects on plants	Plant (corn, Zea mays) heights and shoot wts. were not significantly reduced at 200 ppmw; but at 2000 ppmw DBP, plant height was reduced by 17% and plant shoot wt. by 25%. The low levels (1.24 ppm) of DBP found in plants grown in soil containing 2000 ppmw (Shea et al. 1982). DP affected soybean germination at 200 ppm (dry soil basis) (Overcash et al. 1982). Induces chlorosis in green leafs (Lökke & Rasmussen 1983).	
Effects on wastewater treatment	May flog filters and exchange beds (Sax 1986).	
EC50 values to microorganism, mg/l	10.9	Microtox (Tarkpea et al. 1986)
LC50 values to algae, mg/l	0.02–0.6	(96hr, Gymnodium breve (Wilson et al. 1978)
EC50 values to algae, mg/l	> 3	Chlorella (Melin & Agneus 1983)
	0.75	96hr, Selenastrum (Cox & Moran 1984)
	0.5–0.7 > 0.7	14–22 permillage Skeletonema 27 permillage, Skeletonema (Medlin 1980)
	0.1	96hr, Gymnodinium, grw (Wilson et al. 1978)
LC50 values to crustaceans, mg/l	0.1–1.0 10–50	17d, Palaemonetes pugio, larvae 24hr, Palaemonetes pugio (Laughlin et al. 1978)
	1.7	96hr, Nitocra (Linden et al. 1979)
	2.1	96hr, Gammarus pseudolimnaeus (Mayer & Sanders 1973)
	> 10 2.1	96hr, crayfish 96hr, scud (Sax 1986)
EC50 values to crustaceans, mg/l	3.4	48hr, Daphnia magna (Cox & Moran 1984)
LC50 values to fishes, mg/l	1.2	96hr, Lepomis macrochirus (Buccafusco et al. 1981)
	3 0.92 1.6 0.85	96hr, static, Pimephales 96hr, dynamic, Pimephales 96hr, dynamic, Salmo gairdneri 96hr, static, Lepomis (Cox & Moran 1984)
	4.3	48hr, Orizias latipes (Yoshioka et al. 1986)
	1.3 0.73 2.91 6.47	96hr, Pimephales promelas 96hr, Lepomis macrochirus 96hr, Ictalurus punctatus 96hr, Salmo gairdneri (Sax 1986)

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NOEC values to fishes, mg/l	0.56–1.0 Pimephales, embryo-larvae (Cox & Moran 1984)
Other information about water organisms	EC50, 24hr, 2.2 mg/l, rpd, Tetrahymena pyriformis (Yoshioka et al. 1985). EC50, 96hr, 5.8 mg/l, Chironomus sp. (Cox & Moran 1984). Corophium sp., colonisation, 0.34 mg/l (Tagatz et al. 1983). Daphnia, reproduction, reversible effect (Springborn 1984). Daphnia, reproduction (McCarthy & Whitmore 1985).
Other effects on aquatic ecosystems	Microcosmos, 14d, effective concentration, 3.7 mg/l (Tagatz et al. 1983).
Other information	Persistency: Certain bacterial strains will degrade n-butyl phthalate but only when the initial concentrations are low. – Degradation will take place in fresh-water hydrosoil also through the enzymatic action of microorganisms. Anaerobic conditions will slow biodegradation (Sax 1986). Air pollution: There will be no appreciable vapour. At high temperatures, there will be carbon dioxide (Sax 1986).

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699 • Dibutyl tin dilaurate 77-58-7

Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).

700 • Dibutyl tin oxide 818-08-6

Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).

701 • Dibutylamine 111-92-2

Synonyms	n-Dibutylamine
Sumformula of the chemical	C8H19N
Odour	Odour: characteristic: quality: fish, amine Hedonic tone: unpleasant to neutral Threshold Odour Concentration (T.O.C.): absolute recogn.: 0.08 ppm 50% recogn.: 0.27 ppm 100% recogn.: 0.48 ppm Odour Index 100% recogn.: 5479 (Hellmann & Small 1974)
Molecular weight	129.28
Specific gravity (water=1)	0.76
Conversion factor, 1 ppm in air=	5.29 mg/m³
Conversion factor, 1 mg/m³ in air=	0.189 ppm
Water solubility, mg/l	3500 (MITI 1992)
Melting point, °C	-60–-59 (MITI 1992)
Boiling point, °C	159–160 (MITI 1992)
pKa	11.25 (Sangster 1989)

Log octanol/water coefficient, log Pow	2.83	(Sangster 1989)
Total degradation in water	Biodegradation: 94–97% (NH3) by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
LD50 values to mammals in oral exposure, mg/kg	360 500 550	orl-rat (Lewis & Sweet 1984) orl-rat (Patty 1967) orl-rat (McKee & Wolf 1963)
LD50 values to mammals in non-oral exposure, mg/kg	1010	skn-rbt (Lewis & Sweet 1984)
LCLo values to mammals in inhalation exposure, ppm	500	4hr, ihl-rat (Lewis & Sweet 1984)
EC50 values to algae, mg/l	19	rpd, 96hr, Selenastrum capricornutum (Calamari et al. 1982b)
LC50 values to crustaceans, mg/l	160	24hr, Daphnia magna (Calamari et al. 1982b)
LC50 values to fishes, mg/l	5.5	96hr, Salmo gairdneri (Calamari et al. 1980a)

702 • Dibutyldichlorostannane 683-18-1

Sumformula of the chemical	C6H18Cl2Sn	
Molecular weight	303.85	
LD50 values to mammals in oral exposure, mg/kg	100	orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	126 180	unk-rat ivn-mus (Lewis & Sweet 1984)
LDLo values to mammals in oral exposure, mg/kg	680	orl-rbt (Lewis & Sweet 1984)
LDLo values to mammals in non-oral exposure, mg/kg	5 5 10 1360	ivn-rbt ivn-gpg ivn-rat skn-rbt (Lewis & Sweet 1984)
Other information about mammals	LDfr = 62.5 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).	
Effects on the physiology of water organisms	Poecilia reticulata; 0.320 mg/l, 30d, histological effect (presence of physical damage to tissues) (Wester & Canton 1987).	

703 • Dibutylfumarate 105-75-9

LC50 values to fishes, mg/l	0.89 0.88 0.62 0.69 0.48	4d, Carassius auratus 4d, Ictalurus punctatus 4d, Lepomis macrochirus 4d, Pimephales promelas 4d, Salmo gairdneri (Holcombe et al. 1987)

704 • Dibutyltin bis(2-ethylhexoate) 2781-10-4

Other information about mammals	LDfr = 62.5 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

705 • Dibutyltin diacetate 1067-33-0

Other information about mammals	Ldfr = 87.5 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).	
EC50 values to algae, mg/l	0.035	rpd, 72hr, Skeletonema costatum (Walsh et al. 1985)

706 • Dibutyltin difluoride 563-25-7

Synonyms	Di-n-butyltinfluoride	
Other information about mammals	LDfr = 75.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).	
EC50 values to crustaceans, mg/l	0.056	rpd, 72hr, Skeletonema costatum (Walsh et al. 1985)

707 • Dicamba 1918-00-9

Synonyms	3,6-Dichloro-o-acidic acid Banvel Mediben	
Use	Herbicide.	
State and appearance	White crystalline solids.	
Molecular weight	221.04	
Water solubility, mg/l	7900	
Melting point, °C	114–116	
Half-life in soil, days	14	(Li et al. 1990)
LD50 values to mammals in oral exposure, mg/kg	1040 1190	orl-rat orl-mus (Lewis & Sweet 1984)
Effects on plants	4 oz dicamba /acre (= 0.307 kg/ha) sprayed before the 4-leaf stage of wheat and barley caused gross malformation of the stems and leaves, reduced height, delayed maturity and interfered with normal seed development in the main culms. Under lush conditions of the greenhouse similar effects were induced by half this dosage (= 0.154 kg/ha). Root tips of wheat and barley seedlings, germinated in petri plates at various concentrations of dicamba, showed a sharp reduction in the numbers of dividing cells; mitosis was disturbed by as little as 10 ppm of dicamba (Friesen et al. 1964).	
LC50 values to crustaceans, mg/l	3.9	96hr, Gammarus lacustris (Sanders 1969)
NOEC values to crustaceans, mg/l	100 100 100 100 100 100	srv,48hr, Daphnia magna srv,48hr, Gammarus fasciatus srv,48hr, Asellus brevicaudus 48hr, Cypridopsis vidua 48hr, Palaemonetes kadiakensis 48hr, Orconectes nais (Sanders 1970)

LC50 values to fishes, mg/l	20	48hr, Lepomis macrochirus (Hughes & Davis 1962)
	465	96hr, Gambusia affinis (Johnson 1978)
	> 100	96hr, Oncorhynchus kisutch (Lorz et al. 1979)
	135	96hr, Salmo gairdneri (Pesticide Manual 1983)
	135	96hr, Lepomis macrochirus (Pesticide Manual 1983)

708 • Dicaphthoxon

17650-76-9

Other information about mammals	ALD = 42.o mg/kg, act, orl, deer mouse; LDfr = 25 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

709 • Dichlobenil

1194-65-6

Synonyms	2,6-Dichlorobenzonitrile DCB Casoron Decabane	
Sumformula of the chemical	C7H3Cl2N	
Products containing the chemical	Casoron G	
Use	Active ingredient in herbicides.	
Molecular weight	172.01	
Vapour pressure, mmHg	0.0005	25 °C
Water solubility, mg/l	18	20 °C
Melting point, °C	144–145	
Log octanol/water coefficient, log Pow	2.64	(Anon. 1986)
Log soil sorption coefficient, log Kom	2.37	(Sabljic 1987)
LD50 values to mammals in oral exposure, mg/kg	2710	orl-rat
	681	orl-gpg (Lewis & Sweet 1984)
	2056	orl-mus (Sweet 1987)
	3160	orl-rat (Martin 1968)
	> 2460	orl-male-mus (Anon. 1976)
	501	orl-gpg (Martin 1968)
LD50 values to mammals in non-oral exposure, mg/kg	1350	skn-rbt (Lewis & Sweet 1984)
	360	ipr-mus (Sweet 1987)
TDLo values to mammals in non-oral exposure, mg/kg	0.26	ipr-mus, tumorigenic
	0.26	scu mus, tumorigenic (Sweet 1987)
Effects on arthropods	LC50, 7 mg/l, 96hr, Pteronarcys californica (Sanders & Cope 1968) LC50, 7.8 mg/l, 96hr, Tendipedidae LC50, 10.3 mg/l, 96hr, Callibaetes sp. LC50, 13 mg/l, 96hr, Limnephilus LC50, 20.7 mg/l, 96hr, Enallegma (Wilson & Bond 1969)	

Effects on plants	Incubation of segments of barley coleoptile and Sesbania exaltata hypocotyls in 1% sucrose containing 2 ppm dichlobenil inhibited protein synthesis by 26 and 24%, respectively. (Mann et al. 1965)	
EC50 values to algae, mg/l	25	rpd, schr, Phaeodactylum tricornutum (Walsh 1972)
	2.7	96hr, grw, Scenedesmus subspicatus (Geyer et al. 1985)
LC50 values to crustaceans, mg/l	3.7	48hr, Daphnia pulex (Sanders & Cope 1968)
	10	96hr, Gammarus fasciatus (Sanders 1970)
	10	48hr, Daphnia magna (Sanders 1970)
	10	act, Daphnia magna (Kenaga 1979)
	11	96hr, Gammarus lacustris (Sanders 1969)
	8.5	96hr, Hyallella azteca (Wilson & Bond 1969)
	5.8	48hr, Simocephalus serrulatus (Sanders & Cope 1968)
	7.8	48hr, Cypridopsis vidua (Sanders 1970)
	34	48hr, Asellus brevicaudus (Sanders 1970)
	9	48hr, Palaemonetes kadiakensis (Sanders 1970)
	22	48hr, Orconectes nais (Sanders 1970)
EC50 values to crustaceans, mg/l	9.8	48hr, rpd, Daphnia magna (Martin 1968)
LC50 values to fishes, mg/l	22	48hr, Salmo gairdneri
	20	48hr, Lepomis macrochirus (Edwards 1977)
	4.2	96hr, Rasbora heteromorpha (Tooby et al. 1975)
	1.6	10d, Rutilus rutilus (Tooby et al. 1972)
	20	48hr, Lepomis macrochirus (Wilson & Bond 1969)
	9.4	96hr, Ctenopharyngodon idella (Tooby et al. 1980)
	18	48hr, Poecilia reticulata (Pesticide Manual 1983)
	10	act, Lepomis macrochirus
	18	act, Pimephales promelas (Kenaga 1979)

710 • Dichlofluanid 1085-98-9

Use	Fungicide.	
LD50 values to birds in oral exposure, mg/kg	> 100	orl-Agelaius phoeniceus
	> 100	orl-Sturnus vulgaris (Schafer et al. 1983)
LC50 values to fishes, mg/l	1–10	24hr, Carassius auratus (Pesticide Manual 1983)
	1–10	24hr, Poecilia reticulata (Pesticide Manual 1983)

711 • Dichloro difluoro methane 75-71-8

Synonyms	Freon R 12 Fluorocarbon 12	
Sumformula of the chemical	CCl2F2	
Use	Aerosol propellant (forbidden in Sweden 1979), cooling medium, foamy plastic.	
Molecular weight	120.91	
Density, kg/> 1300	1330	20 °C
Water solubility, mg/l	280	25 °C

Melting point, °C	-158 (MITI 1992)
Boiling point, °C	-29.8 (MITI 1992)
Log octanol/water coefficient, log Pow	2.16
Henry's law constant, Pa x m³/mol	240000 20 °C 39560 calc. (Yaws et al. 1991)
Mobility	Theoretical distribution: 100% in air (Anon. 1989).
Other reactions in atmosphere	Lifetime in troposphere > 81 years (Cunnold et al. 1983). Average persistance in troposphere, based on the reaction with OH-radicals > 330 years (IMOS 1975). Absorbes UV (< 200 nm) at high layers, molecules break up and form strongly reactive chlorine atoms (IMOS 1975).
Half-life in air, days	38325–61685 105–169 years, estim.
Other information about degradation	Not biodegradable (Anon. 1989). Strongly reactive Cl forms in stratosphere. Reacts with ozone: Cl + 03 →ClO + 02 ClO + 0 →Cl + 02 (Anon. 1989).
Bioconcentration factor, fishes	2.8–8.9 6w, Cyprinus carpio, conc 0.1 mg/l 2.3–10 6w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	> 1000 orl-rat (Verschueren 1983)
Other information about mammals	Ihl-mus, 30 min, LC50, 76 vol %; ham, ihl, 30 min, TCLO, 20 vol % (Lewis & Tatken 1980). Rat, ihl, 90d, 2 of 5 dead, 795 ppm (Verschueren 1983). Dog, NOEL, 2 years, 80 mg/kg, day (Sittig 1980).
EC50 values to crustaceans, mg/l	580 24hr, Daphnia (Rippen 1988)
LC50 values to fishes, mg/l	67 48hr, Oryzias latipes (MITI 1992)
Other information	Estimated amount in troposphere; 6,1 Mt (1980), which equals to 19% or the total amount of chlorine bind to organic material (Fabian 1986).

712 • 4,4'-Dichloro-α-(trichloromethyl)benzhydrol

115-32-2

Synonyms	1,1-Bis(p-chlorophenyl)-2,2,2-trichloroethanol 1,1-Bis(4-chlorophenyl)-2,2,2-trichloroethanol 4-Chloro-α-(4-chlorophenyl)-α-(trichloromethyl)benzene-methanol Carbax Dicofol Kelthane
Sumformula of the chemical	C14H9Cl5O
Use	Pesticide, acaricide.
Molecular weight	370.48
Water solubility, mg/l	1.2 24 °C

Melting point, °C	350 (MITI 1992)
Hydrolysis in base	Hydrolysis to DBP at pH 8.2: half-life 60 min. (initial concentration 0.4 mg/l) (Verschueren 1983).
Total degradation in water	Biodegradation: 0% by BOD period: 14D substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	1100–10000 8w, Cyprinus carpio, conc 0.01 mg/l 1600–5100 8w, Cyprinus carpio, conc 0.001 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be accumulated on a medium level (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	575 orl-rat 420 orl-mus 1810 orl-gpg (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	100 skn-rat 1150 ipr-rat 1870 skn-rbt (Lewis & Sweet 1984)
Carcinogenicity	NCI carcinogenesis bioassay completed: results positive, mus; results negative, rat (Lewis & Sweet 1984).
LC50 values to crustaceans, mg/l	3.8 Daphnia pulex (Nishiuchi & Hashimoto 1967) 0.59 48hr, Crangon franciscorum (Khorram & Knight 1977)
LC50 values to fishes, mg/l	0.21 96hr, Salmo gairdneri 0.51 96hr, Pimephales promelas (Holcombe et al. 1982) 0.36 48hr, Cyprinus carpio (Nishiuchi & Hashimoto 1967) 1.14 48hr, Oryzias latipes (MITI 1992)
LOEC values to fishes, mg/l	0.039 srv, schr, Pimephales promelas (Spehar et al. 1982)
NOEC values to fishes, mg/l	0.019 srv, schr, Pimephales promelas (Spehar et al. 1982)
Other information about water organisms	Paramecium aurelia; 1 mg/l; 0.06 d, 100% mortality or 0% survival including algicidal and herbicidal effects (Joshi & Misra 1986).

713 • 4,5-Dichloro-1,2-dithiol-3-one 1192-52-5

Synonyms	Dithiol RYH-86 5-Oxo-3,4-dichloro-1,2-dithiol 4,5-Dichloro-3-oxo-1,2-dithiol 4,5-Dichloro-1,2-dithiocyclopenten-3-one 4,5-Dichloro-3H-1,2-dithiol-3-one
Sumformula of the chemical	C3Cl2OS2
EINECS-number	2147545
Products containing the chemical	Daracide 7816
Purity, %	99–100% (WPSREG 1994)

Known impurities	sulphur 0.1% water 0.04% (WPSREG 1994).
Use	Active substance in slimicides: to prevent slime and clogging caused by harmful micro-organisms in cooling and circulating water systems and paper production (WPSREG 1994).
State and appearance	solid; chrystalline powder (WPSREG 1994).
Molecular weight	185.88
Density, kg/> 1300	1.99 (WPSREG 1994)
Vapour pressure, mmHg	0.012 1.5 Pa (25 °C) 0.033 4.4 Pa (35 °C) 0.083 11 Pa (45 °CC) 0.248 33 Pa (55 °C) (WPSREG 1994)
Water solubility, mg/l	500 about 50 mg/100 ml, 25 °C (WPSREG 1994)
Melting point, °C	58.5–59.5 (technical substance: 57.5–58.7 °C) (WPSREG 1994)
Boiling point, °C	125 1.5 kPa 87 67 Pa (WPSREG 1994)
Flashing point, °C	> 110 °C (WPSREG 1994)
Log octanol/water coefficient, log Pow	3.3–3.9 (WPSREG 1994)
Other physicochemical properties	Solubility in organic solvens: methanol 8% (weight) ethanol 14% (weight) isopropanol 12% (weight) hexane 7% (weight) methylcarbitole 30% (weight) diethylenglycole 20% (weight) Very soluble in acetone, methylcellosolv, toluene, butylacetate and chloroform (WPSREG 1994). Not oxidizing (WPSREG 1994).
Photochemical degradation in water	Primary degradation: T1/2 = 8.4min, pH 5, 25 °C (WPSREG 1994)
Hydrolysis in water	T1/2 = 182hr, pH 6, 37 °C, T1/2 = 0.54hr - 4h, pH 7, 37 °C, T1/2 = 104.4hr, pH 7, 37 °C, (WPSREG 1994).
Hydrolysis in acid	T1/2 = 592hr, pH 4, 37 °C, T1/2 = 54.1d, pH 5, 37 °C, (WPSREG 1994).
Hydrolysis in base	T1/2 = 0.22hr, pH 9, 37 °C, T1/2 = 0.9hr, pH 9, 37 °C, (WPSREG 1994).
Aerobic degradation in water	Primary degradation: T1/2 = 4.2hr, aerobic, pH 7.9–8.8, 24-26 °C (WPSREG 1994).
Degradation and transformation products	2-butanone (CAS 78-93-3) chloranil (CAS 118-75-2) (WPSREG 1994).
LD50 values to mammals in oral exposure, mg/kg	120-372 mg/kg, orl-rat (WPSREG 1994)

D

Other information about mammals	orl-rat, no effects with 7.5 mg kg-1d-1, 3mo (WPSREG 1994).	
EC50 values to algae, mg/l	17 13	ErC50, 0-72hr EbC50, 0-72hr (WPSREG 1994)
NOEC values to algae, mg/l	5.6	72hr, pH 3.8–8.4, nominal concentrations (WPSREG 1994)
LC50 values to crustaceans, mg/l	0.011	Daphnia magna, 48hr, flow-through-test measured concentrations, pH 8.0–8.2, 18–21 °C (WPSREG 1994)
EC50 values to crustaceans, mg/l	0.7 0.45 0.17	Daphnia magna, 24hr, static test, nominal concentrations, pH 7.5–7.9, 21 °C semistatic test, nominal concentrations, 5d, pH 8.1–9.0, 21 °C Daphnia magna, 16d, decrease of reproduction (WPSREG 1994)
LOEC values to crustaceans, mg/l	< 0.056	Daphnia magna, 16d, decrease of reproduction (WPSREG 1994)
NOEC values to crustaceans, mg/l	< 0.018	Daphnia magna, 16d, semistatic test, nominal concentrations, pH 8.1–9.0, 19-21 °C (WPSREG 1994)
LC50 values to fishes, mg/l	0.014 0.018	Salmo gairdneri, 96hr, flow-through-test, measured concentrations, pH 7.7–7.8, 12–13 °C Lepomis macrochirus, 96hr, flow-through-test, measured concentrations, pH 7.6–7.8, 22 °C (WPSREG 1994)
Other information	EC50, growth = 0.25 mg/l, Lemna minor (7d) NOEC, growth = 0.10 mg/l, Lemna minor (7d) EC50, dead of leaves = 0.32 mg/l (7d) NOEC, dead of leaves = 0.10 mg/l (7d), obviously static test nominal concentrations, pH 6–7, 21 °C (WPSREG 1994) LC100 (96hr) Salmo gairdneri: 0.036 mg/l, flow-through-test, measured concentrations (WPSREG 1994).	

714 • 2,3-Dichloro-1,4-naphthoquinone 117-80-6

Synonyms	2,3-Dichloro-1,4-naphthaquinone 2,3-Dichloro-α-naphthoquinone Dichlone Phygon	
Sumformula of the chemical	C10H4Cl2O2	
Use	Pesticide, fungicide.	
State and appearance	Yellow crystals.	
Molecular weight	227.04	
Water solubility, mg/l	0.1	25 °C
Melting point, °C	193	
LD50 values to mammals in oral exposure, mg/kg	1300	orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	5000	skn-rbt (Lewis & Sweet 1984)
TDLo values to mammals in oral exposure, mg/kg	3300	orl-mus (Lewis & Sweet 1984)

TDLo values to mammals in non-oral exposure, mg/kg	22	scu-mus (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	> 316	orl-Agelaius phoeniceus (Schafer et al. 1983)
LC50 values to crustaceans, mg/l	1.1	96hr, Gammarus lacustris (Sanders 1969)
	0.1	96hr, Gammarus fasciatus
	0.025	48hr, Daphnia magna
	0.12	48hr, Cypridopsis vidua
	0.2	48hr, Asellus brevicaudus
	0.45	48hr, Palaemonetes kadiakensis
	3.2	48hr, Orconectes nais (Sanders 1970)
EC50 values to crustaceans, mg/l	0.014	rpd, 48hr, Daphnia magna (Martin 1968)
LC50 values to fishes, mg/l	0.07	48hr, Lepomis macrochirus (Bond et al. 1960)
	0.12	48hr, Micropterus salmoides (Hughes & Davis 1962)
Other information about water organisms	LC50 (48hr)	0.04 mg/l, eggs, Mercennaria mercennaria
	LC50 (48hr)	0.014 mg/l, eggs, Crassostrea virginia
	LC50 (14d)	0.041 mg/l, Crassostrea virginia (Kemp et al. 1973).

715 • 3,4-Dichloro-1-butene 760-23-6

Sumformula of the chemical	C4H6Cl2	
Boiling point, °C	122	(MITI 1992)
Bioconcentration factor, fishes	0.59–2.11	6w, Cyprinus carpio, conc 0.26 mg/l
	< 0.28–13.34	6w, Cyprinus carpio, conc 0.026 mg/l (MITI 1992)
LC50 values to fishes, mg/l	22.6	48hr, Oryzias latipes (MITI 1992)

716 • 2,4-Dichloro-1-naphthol 2050-76-2

Synonyms	2,4-Dichloro-1-hydroxynaphtalene	
Water solubility, mg/l	< 10	(MITI 1992)
Melting point, °C	107	(MITI 1992)
Log octanol/water coefficient, log Pow	4.23	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.3–4.9	6w, Cyprinus carpio, conc 0.01 mg/l
	< 3.0–42	6w, Cyprinus carpio, conc 0.001 (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	0.87	48hr, Oryzias latipes (MITI 1992)

D

717 • 1,4-Dichloro-2-butene 764-41-0

Synonyms	2-Butylene dichloride 1,4-Dichloro-2-butylene cis-1,4-Dichloro-2-butene trans-1,4-Dichlorobutene 1,4-Dichloro-trans-2-butene
Sumformula of the chemical	C4H6Cl2
Use	Chemical intermediate in the production of chloroprene and hexamethylenediamine.
State and appearance	Colourless liquid.
Odour	Characteristic sweet, pungent odour (Sax 1986).
Molecular weight	124.97
Specific gravity (water=1)	1.112 20 °C 1.183 25 °C
Vapour density (air=1)	4
Melting point, °C	1–3, trans -48
Boiling point, °C	155.5 758 mm 55.5 20 mm
Other physicochemical properties	Insoluble in water; soluble in ethanol, diethyl ether, acetone, benzene and chloroform (Sax 1986). Slowly reacts with water to form hydrochloric acid (Sax 1986).
Other information about metabolism	No food chain concentration potential (Sax 1986).
LD50 values to mammals in oral exposure, mg/kg	89 orl-rat (Sax 1986)
LD50 values to mammals in non-oral exposure, mg/kg	56 ivn-mus 620 skn-rbt (Sax 1986)
LC50 values to mammals in inhalation exposure, ppm	86 4hr, ihl-rat (Sax 1986)
LCLo values to mammals in inhalation exposure, ppm	62 ihl-rat, 4hr (Sax 1986)
TDLo values to mammals in non-oral exposure, mg/kg	150 ipr-mus, 77W-I, tumorigenic 150 scu-mus, 77W-I, tumorigenic (Sax 1986)
TCLo values to mammals in inhalation exposure, ppm	5 ihl-rat, 6hr, 6-15d preg (Sax 1986)
Health effects	Inhalation of vapour irritates nose and throat. Contact with eyes causes irritation and tears. Contact of skin with liquid causes severe blistering and dermatitis. Ingestion causes severe irritation of mouth and stomach (Sax 1986). Skin and eye irritation data: skn, rbt, 10 mg, 24hr, severe; eye, rbt, 20 mg, severe (Sax 1986).
Carcinogenicity	Insufficient evidence to determine carcinogenicity of the trans isomer. Skin application and subcutaneous and intraperitoneal dosing produced low incidences of local sarcomas in female mice (Sax 1986).

Mutagenicity	The trans isomer causes reverse mutations in Salmonella typhimurium TA 100 and is mutagenic to Escherichia coli (Sax 1986). Mutagen data: mmo, sat, 1 mmol/l; mma, sat, 1 mmol/l; sln, dmg, orl, 2 mmol/l, 3D-I (Sax 1986).	
LC50 values to fishes, mg/l	0.09	14 d, Poecilia reticulata (Hermens et al. 1985)

718 • 1,3-Dichloro-2-propanol 96-23-1

Water solubility, mg/l	> 100000 (MITI 1992)	
Chemical oxygen demand, g 02/g	0.84	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.01	5 days (Bridie et al. 1979)
Total degradation in water	Biodegradation: 84, 86, 0% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LC50 values to fishes, mg/l	680	24hr, Carassius auratus (Bridie et al. 1979)

719 • 1-(2',5'-Dichloro-4'-sulfophenyl)-3-methyl-5-pyrazolone 84-57-1

Sumformula of the chemical	C10H8Cl2N2O4S	
EINECS-number	2015417	
Water solubility, mg/l	3200	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 2.8 < 32	6w, Cyprinus carpio, conc 2 mg/l 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
LC50 values to fishes, mg/l	434	48hr, Oryzias latipes (MITI 1992)

720 • 3,3'-Dichloro-4,4'-diamino-diphenylmethane 101-14-4

Sumformula of the chemical	C13H12Cl2N2	
EINECS-number	2029189	
Water solubility, mg/l	0.48	(MITI 1992)
Melting point, °C	108	(MITI 1992)

Log octanol/water coefficient, log Pow	3.91	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	130–398 114–232	8w, Cyprinus carpio, conc 0.05 mg/l 8w, Cyprinus carpio, conc 0.005 mg/l (MITI 1992)
LC50 values to fishes, mg/l	1	48hr, Oryzias latipes (MITI 1992)

D

721 • 1,3-Dichloro-4,6-dinitrobenzene 3698-83-7

LD50 values to birds in oral exposure, mg/kg	> 100	orl-Agelaius phoeniceus (Schafer et al. 1983)
LC50 values to crustaceans, mg/l	> 0.126	96hr, Orconectes nais (Phipps & Holcombe 1985)
LC50 values to fishes, mg/l	0.026 0.028 0.038 0.047 0.028	96hr, Salmo gairdneri 96hr, cat fish (Phipps & Holcombe 1985) 96hr, Pimephales promelas 96hr, Carassius auratus 96hr, Ictalurus punctatus (Phipps & Holcombe)
Other information about water organisms	LC50, > 0.126 mg/l, 96hr, snail (Phipps & Holcombe 1985)	

722 • 1,2-Dichloro-4-nitrobenzene 99-54-7

Synonyms	3,4-Dichloronitrobenzene	
Sumformula of the chemical	$C_6H_3Cl_2NO_2$	
Water solubility, mg/l	3 140	20 °C, almost insoluble (Anon. 1986b) (MITI 1992)
Melting point, °C	40–41	(MITI 1992)
Boiling point, °C	105–107	3 mmHg (MITI 1992)
Log octanol/water coefficient, log Pow	2.99 2.95	(Anon. 1986b) (MITI 1992)
Log soil sorption coefficient, log Kom	2.29	(Sabljic 1987)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	26–59 37–65	8w, Cyprinus carpio, conc 0.05 mg/l, 8w, Cyprinus carpio, conc 0.005 mg/l, (MITI 1992)

Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	643	orl-rat (Anon. 1986b)
EC50 values to microorganism, mg/l	9.6	Microtox (Kaiser & Ribo 1985)
EC50 values to algae, mg/l	10	4d, Scenedesmus sp. (Anon. 1986b)
LC50 values to crustaceans, mg/l	4.9	2d, Daphnia magna (Anon. 1986b)
EC50 values to crustaceans, mg/l	1.6	2d, Daphnia magna (Anon. 1986b)
LC50 values to fishes, mg/l	3.9	4d, Poecilia reticulata (Anon. 1986b)
	7.01	48hr, Oryzias latipes (MITI 1992)
EC50 values to fishes, mg/l	0.39	4d, Poecilia reticulata (Anon. 1986b)

D

723 • 3,3'-Dichloro-5,5'-benzidine disulfonic acid 123251-96-7

Sumformula of the chemical	C12H10O6N2S2Cl2	
Water solubility, mg/l	> 2000 (MITI 1992)	
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.1 < 1.6	6w, Cyprinus carpio, conc 2 mg/l 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
LC50 values to fishes, mg/l	645	48hr, Oryzias latipes (MITI 1992)

724 • 2,4-Dichloro-6-methylphenol 1570-65-6

LC50 values to crustaceans, mg/l	0.43	48hr, Daphnia magna (LeBlanc 1980)
LOEC values to fishes, mg/l	0.36	srv, Cyprinodon variegatus (Ward & Parrish 1980)

725 • 2,4-Dichloro-6-nitrophenol 609-89-2

Water solubility, mg/l	17	(MITI 1992)
Melting point, °C	122	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

Bioconcentration factor, fishes	12–23 < 5.0–36	6w, Cyprinus carpio, conc 0.008 mg/l 6w, Cyprinus carpio, conc 0.0008 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	1.32	48hr, Oryzias latipes (MITI 1992)
Other information about water organisms	Tetrahymena pyriformis; 3.7 mg/l, 2d, EC50, grw (Schultz 1987).	

726 • Dichloro-m-xylene 626-16-4

LC50 values to fishes, mg/l	0.12	14d, Poecilia reticulata (Könemann 1979)

727 • Dichloroacetic acid 79-43-6

Sumformula of the chemical	C2H2O2Cl2	
State and appearance	Colourless liquid	
Odour	Odour threshold: recognition: 0.23 mg/m³	
Molecular weight	129	
Specific gravity (water=1)	1.563	at 20/4 °C
Vapour pressure, mmHg	1	at 44 °C (Verschueren 1983)
Water solubility, mg/l	86300	(Suntio et al. 1988)
Melting point, °C	9.7 5–6 °C	(Weast 1982–83) (Verschueren 1983)
Boiling point, °C	194	
pKa	1.29 1.48	
Log octanol/water coefficient, log Pow	0.76 -0.14–1.39 calc. (Verschueren 1983)	
Henry's law constant, Pa x m³/mol	0.056	calc. (Suntio et al. 1988)
Total degradation in water	Biodegradation: 97% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	4500 5500	orl-rat (Patty 1967) orl-mus (Patty 1967)
LC50 values to crustaceans, mg/l	23	96hr, Nitocra spinipes (Linden et al. 1979)

728 • 2,4-Dichloroacetophenone 2234-16-4

LC50 values to fishes, mg/l	11.7	96hr, Pimephales promelas (Veith et al. 1983)

729 • 2,3-Dichloroaniline 608-27-5

Sumformula of the chemical	C6H5Cl2N
Log octanol/water coefficient, log Pow	2.78 (Anon. 1986)

730 • 2,4-Dichloroaniline 554-00-7

Molecular weight	162.02	
Water solubility, mg/l	0.62	(MITI 1992)
Melting point, °C	60–63	(MITI 1992)
Boiling point, °C	245	(MITI 1992)
Log octanol/water coefficient, log Pow	2.85	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	12–30 15–28	6w, Cyprinus carpio, conc 0.05 mg/l 6w, Cyprinus carpio, conc 0.005 mg/l (MITI 1992)
LDLo values to mammals in oral exposure, mg/kg	113	orl-cat (Lewis & Sweet 1984)
Effects on amphibia	NOEC, 1 mg/l, 100d, Xenopus laevis, mortality. NOEC, 0.32 mg/l, 100d, Xenopus laevis, development. NOEC, 1 mg/l, 100d, Xenopus laevis, growth. (Slooff & Canton 1983)	
Effects on arthropods	NOEC, 10 mg/l, 25d, Culex pipiens, mortality NOEC, 10 mg/l, 25d, Culex pipiens, development. (Slooff & Canton 1983)	
Effects on plants	NOEC, 1 mg/l, 7d, Lemna minor, specific growth rate. (Slooff & Canton 1983)	
Effects on microorganisms	NOEC, 10 mg/l, 0.3d, Pseudomonas fluorescens, specific growth rate. NOEC, 1 mg/l, 4d, Micrcystis aeruginosa, specific growth rate. (Slooff & Canton 1983)	
NOEC values to algae, mg/l	1 3.2	96hr, rpd, Microcystis aeruginosa (Slooff & Canton 1983) 4d, grw (biomass), Scenedesmus pannonicus (Slooff & Canton 1983)
LC50 values to crustaceans, mg/l	0.71 3	48hr, Daphnia magna (Hermens et al. 1984) 21d, Daphnia magna (van Leeuwen et al. 1987)
EC50 values to crustaceans, mg/l	0.08 0.12	17 days, rpd, Daphnia magna (Hermens et al. 1984) Daphnia magna (van Leeuwen et al. 1987)
NOEC values to crustaceans, mg/l	0.032	21 days, srv, Daphnia magna (Slooff & Canton 1983)
LC50 values to fishes, mg/l	6.4 11.7 12.7	14 d, Poecilia reticulata (Hermens et al. 1985) 14 days, Poecilia reticulata (Könemann 1979) 48hr, Oryzias latipes (MITI 1992)

D

NOEC values to fishes, mg/l	3.2	28d, srv, Poecilia reticulata
	1	28d, srv + bhv, Poecilia reticulata
	1	28d, grw, Poecilia reticulata
	0.32	40d, srv, Oryzias latipes
	0.32	40d, srv + bhv, Oryzias latipes
	3.2	40d, grw, Oryzias latipes
		(Slooff & Canton 1983)
Other information about water organisms	EC50 31 mg/l, 24hr, rpd, Tetrahymena pyriformis (Yoshioka et al. 1985). NOEC, 3.2 mg/l, 21d, Hydra oligactis, specific growth rate. NOEC, 3.2 mg/l, 40d, Lymnaea stagnalis, mortality. NOEC, 1 mg/l, 40d, Lymnaea stagnalis, reproduction. NOEC, 3.2 mg/l 40d, Lymnaea stagnalis, hatching. (Slooff & Canton 1983)	

D

731 • 2,5-Dichloroaniline 95-82-9

Melting point, °C	48.2	(MITI 1992)
Boiling point, °C	251	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	7.9–27.0	6w, Cyprinus carpio, conc 0.2 mg/l
	11.1–19.5	6w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	1.7	14 d, Poecilia reticulata (Hermens et al. 1985)
	10.8	48hr, Oryzias latipes (MITI 1992)

732 • 3,4-Dichloroaniline 95-76-1

Synonyms	3,4-DCA 1-Amino-3,4-dichlorobenzene 3,4-Dichlorobenzenamine 4,5-Dichloroaniline	
Sumformula of the chemical	C6H5Cl2N	
Use	Intermediate.	
Molecular weight	162.02	
Log octanol/water coefficient, log Pow	3.35	(Anon. 1988)
Log soil sorption coefficient, log Kom	2.05	(Sabljic 1987)
Henry's law constant, Pa x m³/mol	2.3	(Anon. 1988)

Mobility	Equilibrium distribution: mass % air 37.07 water 46.84 solid 16.09 (Anon. 1988).
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	7.1–14.4 6w, Cyprinus carpio, conc 0.2 mg/l 4.1–13.4 6w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
Other information about mammals	LDfr = 75.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).
LD50 values to birds in oral exposure, mg/kg	237 orl-Agelaius phoeniceus 562 orl-Sturnus vulgaris (Schafer et al. 1983)
LC50 values to fishes, mg/l	9.5 48hr, Poecilia reticulata, juv. (Adema & Vink 1981) 6.3 14 days, Poecilia reticulata (Hermens et al. 1985) 9.03–12.0 1d, Pimephales promelas 8.88–10.0 2d, Pimephales promelas 6.99–8.06 4d, Pimephales promelas (Call et al. 1987a) 13 48hr, Oryzias latipes (MITI 1992)
Effects on the physiology of water organisms	Pimephales promelas; 0.00510 mg/l, 32 d, change in growth (Call et al. 1987a).
Other information about water organisms	EC50 9 mg/l, 24hr, rpd, Tetrahymena pyriformis (Yoshioka et al. 1985).

733 • 3,5-Dichloroaniline 626-43-7

LC50 values to fishes, mg/l	3.9 14 d, Poecilia reticulata (Hermens et al. 1985)

734 • 2,6-Dichlorobenzaldehyde 83-38-5

Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).

735 • 2,6-Dichlorobenzamide 2008-58-4

EC50 values to algae, mg/l	100 grw, act, 4 d, Chlorella pyrenoidosa (Leeuwen & Maas 1985)
LC50 values to crustaceans, mg/l	320 21 d, Daphnia magna (Leeuwen & Maas 1985)
LC50 values to fishes, mg/l	235 4 d, Salmo gairdneri (Leeuwen & Maas 1985)
Other information	Degradation product of dichlobenil.

736 • 1,2-Dichlorobenzene 95-50-1

Synonyms	o-Dichlorobenzene Chloroben Chloroden	
Sumformula of the chemical	$C6H4Cl2$	
Use	Manufacture of 3,4-dichloroaniline; solvent; dye manufacturing; metal polishes; fumigant and insecticide; metal polishes; industrial odour control.	
State and appearance	Colourless liquid.	
Odour	Odour: recognition: 0.12 mg/m³ Threshold Odour Concentration (T. O. C.): avg. 50 ppm = 305 mg/m³ 300 mg/m³ Odour Index (O. I.): at 20 °C = 26 T. O. C. (water) = 0.01 mg/l (Verschueren 1983)	
Molecular weight	147	
Specific gravity (water=1)	1.305	20/4 °C (Verschueren 1983)
Conversion factor, 1 ppm in air=	6.01	mg/m³ (Verschueren 1983)
Conversion factor, 1 mg/m³ in air=	0.116	ppm (Verschueren 1983)
Vapour pressure, mmHg	1 1.5 1.9	20 °C 25 °C 30 °C
Water solubility, mg/l	134 153.9 137 < 10	20 °C (Anon. 1986)b 25 °C (Chiou et al. 1982) 25 °C (Banerjee 1984) (MITI 1992)
Melting point, °C	-17	(Suntio et al. 1988)
Boiling point, °C	180.5 180.5	(Anon. 1986)b (MITI 1992)
Log octanol/water coefficient, log Pow	3.36 3.38 3.38 3.38 3.59 3.55 3.4 3.38 3.4 3.38	(Chin et al. 1986) (Anon. 1986)b (Anon. 1988) (Hansch & Leo 1979) (Yalkowsky 1979) (Konemann et al. 1979) (Banerjee et al. 1980) (Miller et al. 1984) (Wateral et al. 1982) (Verschueren 1983)
Henry's law constant, Pa x m³/mol	320 193 299	(Anon. 1988) exptl. (Suntio et al. 1988) calc. (Yaws et al. 1991)
Volatilization	Relative volatility (nBuAc=1) = 0.13	
Mobility	Equilibrium distribution: air water solid	 *mass %* 98.77 0.90 0.33 (Anon. 1988).

Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Other information about degradation	Degradation by Pseudomonas (200 mg/l): Parent: 100% ring disruption in 72hr Mutant: 100% ring disruption in 26hr (Verschueren 1983) Degradation of 1,2-dichlorobenzene:

ENVIRONMENT	*INIT.CONC. mg/l*	*REDOX-COND.*	*TEMP. °C*	*DEGRADATION %/day*	*REF.*
water	200	aerobic	30	100/72	a
water	5	aerobic	25	45/7	b
water	10	aerobic	25	20/7	b
water (adapted)	5	aerobic	25	29/7	b
water (adapted)	10	aerobic	25	18/7	b
groundwater	0.01	aerobic	-	97/20	c
groundwater	0.01	sulfate reducing	-	0/1000	c
groundwater	0.01	nitrate reducing	-	0/1000	c
groundwater	0.01	methanogen	-	0/1000	c
soil	0.04	aerobic	-	20/18	d

a) Verschueren 1983 b) Tabak et al. 1981
c) Bouwer 1987 d) Zehnder 1984

Bioconcentration factor, fishes	89	14d, Lepomis macrochirus (Anon. 1986b)
	150–230	8w, Cyprinus carpio, conc 0.1 mg/l
	90–260	8w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon.1987).	
LD50 values to mammals in oral exposure, mg/kg	500	orl-rat
	500	orl-rbt (Lewis & Sweet 1984)
	4386	orl-mus (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	840	ipr-rat (Sweet 1987)
LDLo values to mammals in oral exposure, mg/kg	2000	orl-gpg (Sweet 1987)
LDLo values to mammals in non-oral exposure, mg/kg	400	ivn-mus
	250	ivn-rbt (Sweet 1987)
LCLo values to mammals in inhalation exposure, ppm	800	ihl-gpg, 24hr (Sweet 1987) ihl-rat, 7hr
	821	ihl-gpg, 24hr (Sweet 1987) ihl-rat, 7hr
TDLo values to mammals in non-oral exposure, mg/kg	50	ipr-rat, rpd, paternal effects (Sweet 1987)
TCLo values to mammals in inhalation exposure, ppm	200	ihl-rat, 6hr, rpd, specific developmental abnormalities (Sweet 1987)

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Health effects	Man: severe toxic effects: 300 ppm = 1836 mg/m³, 60 min symptoms of illness: 100 ppm = 612 mg/m³ unsatisfactory: 25 ppm = 153 mg/m³ strong and irritating odour: 100 ppm no injury at average: 15 ppm range: 1–44 ppm (Verschueren 1983)	
Carcinogenicity	NTP carcinogenesis studies; no evidence: mouse, rat (Sweet 1987).	
Effects on microorganisms	EC50, Photobacterium phosphreum, 4,0 mg/l, 30 min (Anon. 1986b) Toxicity threshold (cell multiplication inhibition test): Pseudomonas putida: 15 mg/l (Bringmann & Kühn 1980a)	
EC50 values to microorganism, mg/l	280	0.5hr, Resazurin reduction, methanol
	280	0.5hr, Resazurin reduction, ethanol
	240	0.5hr, Resazurin reduction, acetone
	400	0.5hr, Resazurin reduction, DMSO (Thompson 1986)
EC50 values to algae, mg/l	91.6	96hr, Selenastrum capicornutum chlorophyll a (Anon. 1986)b
	98	96hr, Selenastrum capicornutum cellnumber (Anon. 1986)b
	2.2	96hr, growth, Selenastrum capricornutum
	10	3h, photosynthesis, Selenastrum capricornutum (Calamari et al. 1983)
LOEC values to algae, mg/l	53	Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to crustaceans, mg/l	9.4	96hr, Palaemonetes pugio (Curtis et al. 1979)
	2.4	48hr, Daphnia magna (LeBlanc 1980)
	2.44	Daphnia magna (Anon. 1986b)
	11.76	Tanytarsus dissimilis (Anon. 1986b)
	0.78	24hr, Daphnia magna (Calamari et al. 1983)
EC50 values to crustaceans, mg/l	0.78	24hr, srv, Daphnia magna (Calamari et al. 1983)
	45	24hr, Daphnia magna (Anon. 1986)b
LC50 values to fishes, mg/l	5.6	96hr, Lepomis macrochirus (Buccafusco et al. 1981)
	7.3	96hr, Menidia beryllina
	7.3	96hr, Menidia audens
	27	96hr, Lepomis macrochirus (Dawson et al. 1977)a
	5.9	14 days, Poecilia reticulata (Könemann 1979)
	57	96hr, Pimephales promelas
	9.4	96hr, Palaemonetes pugio (Curtis et al. 1979)
	29	48hr, 29/20 mg/l, Leuciscus idus
	20	melanotus
	1.58	Salmo gairdneri
	27	Lepomis macrochirus
	5.59	Lepomis macrochirus (Anon. 1986)b
	2.3	48hr, Salmo gairdneri
	6.8	48hr, Brachydadio rerio (Calamari et al. 1983)
	1.61	96hr, Salmo gairdneri (USEPA 1984)
	10	48hr, Oryzias latipes (MITI 1992)

EC50 values to fishes, mg/l	1.55 96hr, Salmo gairdneri (USEPA 1984)
Other information about water organisms	EC50 51 mg/l, 24hr, rpd, Tetrahymena pyriformis (Yoshioka et al. 1985). Toxicity threshold (cell multiplication inhibition test): Microcystis aeruginosa 53 mg/l (Bringmann & Kühn 1976) Scenedesmus quadricauda > 100 mg/l (Bringmann & Kühn 1980a) Entosiphon sulcatum > 64 mg/l (Bringmann & Kühn 1980a) Uronema parduczi Chatton-Lwoff 80 mg/l (Bringmann & Kühn 1980b)

737 • 1,3-Dichlorobenzene

541-73-1

Synonyms	m-Dichlorobenzene m-Phenylenedichloride
Sumformula of the chemical	C6H4Cl2
Use	Byproduct. Fumigant and insecticide. Occurs as an impurity in 1,2-dichlorobenzene.
State and appearance	Colourless liquid, denser than and insoluble in water.
Odour	Medium odour threshold; 0.02 ppm (Sax 1986).
Molecular weight	147
Specific gravity (water=1)	1.2884 20/4 °C
Vapour density (air=1)	5.08
Vapour pressure, mmHg	1
Water solubility, mg/l	134.1 25 °C (Chiou et al. 1982) 133.5 25 °C (Banerjee et al. 1980) 124.5 25 °C (Miller et al. 1984) 83 (MITI 1992)
Melting point, °C	-24.7 (Suntio et al. 1988) -24.4 (MITI 1992)
Boiling point, °C	172 (MITI 1992)
Log octanol/water coefficient, log Pow	3.24–3.60 (Sabljic 1987) 3.48 (Anon. 1988) 3.38 (Hansch & Leo 1979) 3.59 (Yalkowsky 1979) 3.6 (Konemann et al. 1979) 3.44 (Banerjee et al. 1980) 3.48 (Miller et al. 1984) 3.53 (Wateral et al. 1982) 3.38 (Verschueren 1983) 3.72 (MITI 1992)
Henry's law constant, Pa x m³/mol	640 (Anon. 1988) 376.1 calc. (Suntio et al. 1988) 328.4 calc. (Yaws et al. 1991)
Mobility	Equilibrium distribution: *mass %* air 99.36 water 0.44 solid 0.21 (Anon. 1988)

Other physicochemical properties	Can react violently with aluminum. Can react vigorously with oxidizing materials. Flammability: moderate. Does not ignite readily. Practically insoluble. Soluble in alcohol and ether. – Soluble in benzene, ligroine, and carbon tetrachloride.
Other chemical degradation processes	1,3-dichlorobenzene is not anticipated to undergo hydrolysis at an appreciable rate under environmental conditions. Sorption processes may be substantial for pollutant concentration anticipated in environmental waters. It will presumably be absorbed by sedimentary organic material (Sax 1986).
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Other information about degradation	Degradation by Pseudomonas (200 mg/l), 30°C: Parent: 100 % ring disruption in 96 hr Mutant: 100 % ring disruption in 28 hr (Verschueren 1983)

Degradation of 1,3-dichlorobenzene:

ENVIRONMENT	*INIT.CONC. mg/l*	*REDOX-COND.*	*TEMP. °C*	*DEGRADATION %/day*	*REF.*
water	200	aerobic	30	100/96	a
water	5	aerobic	25	59/7	b
water	10	aerobic	25	58/7	b
water (adapted)	5	aerobic	25	35/7	b
water (adapted)	10	aerobic	25	33/7	b
groundwater	0.01	aerobic	-	71/500	c
groundwater	0.01	sulfate reducing	-	0/1000	c
groundwater	0.01	nitrate reducing	-	0/1000	c
groundwater	0.0	methanogen	-	0/1000	c

a) Verschueren 1983　c) Bouwer 1987
b) Tabak et al. 1981　d) Zehnder 1984

The estimated atmosperic residence time of dichlorobenzene is 39 days. The compounds react with the hydroxyl radical, photolysis is possible, and physical removal is unlikely. Anticipated products are chlorinated phenols, ring cleavage products, and nitro compounds. – 1,3-dichlorobenzene is probably very persistent and will probably be biodegraded only very slowly by microorganisms already growing on another hydrocarbon source. Atmospheric processes are expected to regulate the fate of 1,3-dichlorobenzene when volatilization occurs at a more rapid rate than sorption or bioaccumulation. If the latter processes are faster than volatilization, biodegradation by aquatic microorganisms is expected to control its fate. It is expected to evaporate from solutions in water within 4 hours if the water is aerated and within 3 days if unaerated (Sax 1986).

Metabolism in mammals	Administration of 1,3-dichlorobenzene to rabbits yielded N-acetyl-s-(2,4-dichlorophenyl)-L-cysteine, 2,4-dichlorophenol and 3,5-dichlorophenol (Sax 1986). When fed to rabbits, m-dichlorobenxene yielded glucuronides (31 %), sulfates (11%), mercapturic acid (9%) and catechols (4 %). In addition, 2,4-dichlorophenylmercapturic acid and 3,5-dichlorocatechol were also observed (Sax 1986).
Other information about metabolism	The weighted average bioconcentration factor for 1,3-dichlorobenzene and the edible portion of all freshwater and estuarine aquatic organisms consumed by Americans is calculated to be 41.2. Dichlorobenzenes concentrate in abdominal and renal adipose tissue as evidenced by human autopsy findings and rat drinking water studies. Toxic effects caused by absorbed dichlorobenzenes indicate distribution to at least the brain, heart, liver, kidney, and bone marrow in many mammalian species. Excretion is relatively slow. Rabbits given a single intragastric dose of 500 mg/kg excreted all of the 1,3-dichlorobenzene and its metabolites within 5 days (Sax 1986).

Bioconcentration factor, fishes	66	14d, whole body, Lepomis macrochirus (Sax 1986)
	97	32d, Pimephales promelas (USEPA 1984)
	57–229	8w, Cyprinus carpio, conc 0.1 mg/l
	58–370	8w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
Health effects	Exposure to dichlorobenzenes will aggravate existing liver damage (Sax 1986). Direct contact: Eye, skin, and mucous membrane irritation. May cause burning eyes, flow of tears, coughing, difficult breathing (Sax 1986). General sensation: Headache, drowsiness, unsteadiness. If individual is intoxicated, effects should disappear after exposure to fresh air for approximately 10 minutes (Sax 1986). Acute hazard level: Irritant. Inhalation of vapour extremely irritating. Brief exposure effects last only a few minutes. Exposure in an enclosed area may be very harmful. – May be absorbed after inhalation, ingestion, or skin contact. Chronic hazard level: Persons exposed chronically to vapours of dichlorobenzene mixtures including 2% 1,3-dichlorobenzene have developed leukemia (Sax 1986).	
Carcinogenicity	Dichlorobenzenes are suspected of playing a role in human leukemia (Sax 1986).	
Mutagenicity	Treating the soil mold organism Aspergillus nidulans for one hour with an ether solution of 1,2-, 1,3-, and 1,4-dichlorobenzene isomers increased the frequency of back-mutations (Sax 1986).	
Teratogenicity	Teratogenicity of dichlorobenzenes has not been studied, but the potential for transplacental toxicosis or developmental effecs may be inferred from evidence that lower chlorinated benzenes pass membrane barriers and affect hormone-metabolizing systems (Sax 1986).	
Effects on wastewater treatment	Degradation by Pseudomonas at 200 ppm at 30 °C parent; 100% ring disruption in 96 hours, mutant; 100% ring disruption in 28 hours. – In wastewater significant biodegradation occurred with gradual adaption followed by a de-adaptive process in subsequent subcultures (Sax 1986).	
EC50 values to microorganism, mg/l	3.3	15 min Microtox (Hermens et al. 1985)
	160	0.5hr, Resazurin reduction, methanol
	150	0.5hr, Resazurin reduction, ethanol
	200	0.5hr, Resazurin reduction, acetone
	170	0.5hr, Resazurin reduction, DMSO (Thompson et al. 1986)
EC50 values to algae, mg/l	179	96hr, Selenastrum capricornutum chlorophyll A
	149	96hr, Selenastrum capricornutum cell number
	52.8	96hr, Skeletonema costatum chlorophyll A
	49.6	96hr, Skeletonema costatum cell number (Sax 1986)
LC50 values to crustaceans, mg/l	1.7	48hr, Daphnia magna (Hermens et al. 1984)
	28	48hr, Daphnia magna (LeBlanc 1980)
	28.1	48hr, Daphnia magna
	2.85	96hr, Mysidopsis bahia (Sax 1986)
	7.43	48hr, unfed, Daphnia magna
	7.23	48hr, fed, Daphnia magna (USEPA 1984)

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EC50 values to crustaceans, mg/l	1.4	16 days, rpd, Daphnia magna (Hermens et al. 1984)
	0.95	16 d, grw, Daphnia magna (Deneer et al. 1988)
	4.23	48hr, unfed, Daphnia magna
	5.98	48hr, fed, Daphnia magna (USEPA 1984)
NOEC values to crustaceans, mg/l	0.689–1.45	28d, Daphnia (USEPA 1984)
LC50 values to fishes, mg/l	5	96hr, Lepomis macrochirus (Buccafusco et al. 1981)
	7.4	14 days, Poecilia reticulata (Könemann 1979)
	7.8	96hr, Pimephales promelas (Veith et al. 1983)
	33.7	96hr, Pimephales promelas (Curtis et al. 1979)
	9.12	96hr, Pimephales promelas (Broderius & Kahl 1985)
	7.8	4d, Pimephales promelas (Carlson & Kosian 1987)
	7.79	96hr, Pimephales promelas
	5	96hr, Lepomis macrochirus
	22	24hr, Lepomis macrochirus, young
	7.77	96hr, Cyprinodon variegatus (Sax 1986)
	12.7	96hr, Pimephales promelas (Curtis & Ward 1981)
	7.79	96hr, flow-through, Pimephales promelas
	1.61	96hr, Salmo gairdneri (USEPA 1984)
	9	48hr, Oryzias latipes (MITI 1992)
NOEC values to fishes, mg/l	1.0–2.267	32d, Pimephales promelas (USEPA 1984)
Other information about water organisms	EC50 130 mg/l, 24hr, rpd, Tetrahymena pyriformis (Yoshioka et al. 1985).	

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Synonyms	p-Dichlorobenzene	
Sumformula of the chemical	C6H4Cl2	
Use	Manufacturing repellents, air deodourizers, dyes and intermediates; manufacturing pharmaceuticals; active ingredient in insecticides, soil fumigant.	
State and appearance	Colourless or white crystals only slightly soluble in water.	
Odour	Very distinctive aromatic, mothball like odour. Odour threshold: lower: 15 to 30 ppm (Sax 1980). Odour Index: at 20 °C = 26 (Verschueren 1983)	
Molecular weight	147	
Specific gravity (water=1)	1.4582	20.5/4 °C
Vapour density (air=1)	5.08	
Density, kg/m³	1250	20 °C
Vapour pressure, mmHg	0.6	20 °C
Water solubility, mg/l	80–87	25 °C
	87	(Anon. 1989)
	65.3	25 °C (Banerjee 1984)
Melting point, °C	53.1	(Suntio et al. 1988)
Boiling point, °C	173	(Anon. 1986b)

Log octanol/water coefficient, log Pow	2.4 (Anon.1989) 3.39 (Anon. 1986) 3.37 (Anon. 1988) 3.38 (Schwarzenbach et al. 1983) 3.38 (Hansch & Leo 1979) 3.59 (Yalkowsky et al. 1979) 3.62 (Konemann et al. 1979) 3.24 (Mackay et al. 1979) 3.52 (Wateral et al. 1982) 3.38 (Miller et al. 1984) 3.37 (Banerjee et al. 1980) 3.39 at 20 °C (Verschueren 1983) 3.53 (Mackay 1982)
Henry's law constant, Pa x m³/mol	380 (Anon. 1988) 240 exptl. (Suntio et al. 1988) 438.5 calc. (Yaws et al. 1991)
Mobility	Equilibrium distribution: *mass %* air 98.98 water 0.75 solid 0.27 (Anon. 1988).
Other physicochemical properties	Theoretical distribution: > 97% in atmosphere (Nordic 1988). Flammability: moderate; flammable hazard when exposed to heat, flame or oxidizers (Sax 1986). Resistant to autooxidation by the peroxy radical in water. Reactive to hydroxyl radicals in air. Will probably not hydrolize in ambient waters due to extreme difficulty in undergoing nucleophilic substitution. Relatively rapid volatilization. Log octanol/water partition coefficient = 3.39 indicated sorption processes substantial at pollutant concentrations anticipated in environmental waters (Sax 1986).
Photochemical degradation in air	Photochemical degradation very unlikely in practice (Jori et al. 1982).
Other reactions in atmosphere	In sunlight (> 300 nm), forming of 2,5,4'-trichlorobiphenyl (Uyeta et al. 1976). Combined effect of UV and NOx – forming of dichloronitrobenzene, dichlorophenol, dichloronitrophenol (Nojima & Kanno 1980).
Aerobic degradation in soil	Many studies indicate that 1,4-dichlorobenzene is easily biodegradable in soil in aerobic conditions after the adaption of microflora (Tabak et al. 1981).
Aerobic degradation in water	In water aerobic degradation is relatively fast but inhibition of bacteria takes place at 5–10 mg/l (Tabak et al. 1981).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
Other information about degradation	Degradation by Pseudomonas (200 mg/l, 30 °C): Parent: 100% ring disruption in 92hr Mutant: 100% ring disruption in 25hr (Verschueren 1983)

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	Degradation of 1,4-dichlorobenzene:

ENVIRONMENT	*INIT.CONC. mg/l*	*REDOX-COND.*	*TEMP. °C*	*DEGRADATION %/day*	*REF.*
water	200	aerobic	30	100/92	a
water	5	aerobic	25	55/7	b
water	10	aerobic	25	37/7	b
water (adapted)	5	aerobic	25	16/7	b
water (adapted)	10	aerobic	25	0/7	b
groundwater	0.01	aerobic	-	99/10	c
groundwater	0.01	sulfate reducing	-	0/1000	c
groundwater	0.01	nitrate reducing	-	0/1000	c
groundwater	0.01	methanogen	-	0/1000	c
soil	0.00023	aerobic	-	> 95/50	d
soil	0.04	aerobic	-	90/18	d
soil	0.0003	aerobic	20	100/50	e
soil	0.06	nitrate reducing	20	0/90	e
soil	0.00024	nitrate reducing	20	100/90	f
soil (adapted)	0.00024	aerobic	20	84/28	f

a) Verschueren 1983 b) Tabak et al. 1981
c) Bouwer 1987 d) Zehnder 1984
e) Kuhn et al. 1985 f) Hutchins & Ward 1984

Chemical degradation: forming of p-chlorophenyl radicals (Shimoda et al. 1979).

Persistant in anaerobic conditions, also in aerobic conditions lag phase is long (Kaare Jensen et al. 1987).

Lag phase (Calamari et al. 1982a).

Degradation products of special interest: dichloroanisoles from dichlorophenols (bacteria) (Allard et al. 1987).

Metabolism in mammals	1,4-dichlorobenzene is quickly absorbed in alimentary canal and is accumulated mainly in fat tissue. – 1,4-dichlorobenzene is metabolized to 2,5-dichlorophenol and is excreted in urine as glukoronides (Jori et al. 1982).
Bioconcentration factor, fishes	214–1800 (Verschueren 1983) 60 14d, Lepomis macrochirus 116 10d, Brachydanio rerio 346 10d, Salmo gairdneri (Anon. 1986b) 218 Salmo gairdneri (Neely 1979) 60–100 Poecilia (Könemann 1979) 60 Lepomis (USEPA 1979) 112 32d, Pimephales promelas (USEPA 1984) 1800 Poecilia reticulata (Neely et al. 1974)
Bioconcentration factor, other organisms	20 (Verschueren 1983) 20 Sidero capsa treubii (Könemann 1979)
LD50 values to mammals in oral exposure, mg/kg	500 orl-rat 2950 orl-mus (Lewis & Sweet 1984) 500 orl-rat (Anon. 1986b)
LD50 values to mammals in non-oral exposure, mg/kg	2562 ipr-rat 5145 scu-mus (Sax 1986)
LDLo values to mammals in oral exposure, mg/kg	2800 orl-gpg (Sax 1986)

TDLo values to mammals in oral exposure, mg/kg	330	orl-ham (Lewis & Sweet 1984)
	300	orl-man (Jori et al. 1982)
Other information about mammals	Rat, ihl, 8 h/day, 5 d/w, 12 w, 798 ppm– 2 of 19 dead, liver necrosis, eye irritation (Hollingsworth et al. 1956).	
Health effects	Has been reported to cause liver injury in humans. Target organs are liver, respiratory system, eyes, kidneys, skin (Sax 1986). Painful to eyes and nose at 50 to 80 ppm, severe discomfort at 160 ppm; very little irritation to skin (Sax 1986). General sensation: headache; eye irritation and swelling; inflammation of nose; anorexia; nausea; vomiting; weight loss; jaundice; cirrhosis (Sax 1986). Skin and eye irritation data: eye, hmn, 80 ppm (Sax 1986).	
Carcinogenicity	In a 2 year study: increased tumout frequence in kidneys and liver (Fawell & Hunt 1988).	
Mutagenicity	Negative in Ames test (Fawell & Hunt 1988). Mutagen data: mmo, asn, 200 mg/l (Sax 1986).	
Teratogenicity	Teratogenicity of DCB has not been studied but potential for transplacental toxicosis or developmental effects may be inferred from evidence that lower chlorinated benzenes pass membrane barriers and affect hormone-metabolizing systems (Sax 1986).	
Other information about birds	Goose, mortality after 600 mg/kg in day, 28 days: 30% (Hollingsworth et al. 1956).	
Effects on microorganisms	EC50, Photobacterium phosphoreum, 5.3 mg/l, 30 min (Anon. 1986b)	
EC50 values to microorganism, mg/l	180	0.5hr, Resazurin reduction, methanol
	190	0.5hr, Resazurin reduction, ethanol
	290	0.5hr, Resazurin reduction, acetone
	220	0.5hr, Resazurin reduction, DMSO (Thompson et al. 1986)
LC50 values to algae, mg/l	1.6	rpd, 96hr, Selenastrum capricornutum (Calamari et al. 1982a)
EC50 values to algae, mg/l	98.1	96hr, Selenastrum capricornutum chlorophyll a
	96.7	96hr, Selenastrum capricornutum cellnumber (Anon. 1986b)
	54.8	96hr, Skeletonema costatum chlorophyll a
	59.1	96hr, Skeletonema costatum cellnumber (Sax 1986)
	0.1	96hr (Sax 1986)
	1.6	96hr, growth, Selenastrum capricornutum
	5.2	3h, photosynthesis, Selenastrum capricornutum (Calamari et al. 1983)
LC50 values to crustaceans, mg/l	1.6	24hr, Daphnia magna (Calamari et al. 1982a)
	69	96hr, Palaemonetes pugio (Curtis et al. 1979)
	11	48hr, Daphnia magna (LeBlanc 1980)
	11	48hr, Daphnia magna
	1.6	24hr, Daphnia magna
	13	Tanytarsys dissimilis (Anon. 1986b)
	0.2	96hr, Mysidopsis (Sax 1986)
	1.6	24hr, Daphnia magna (Calamari et al. 1983)
EC50 values to crustaceans, mg/l	1.6	24hr, Daphnia (Calamari et al. 1982a)
	3.5	48hr, Daphnia (Abernethy et al. 1986)

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NOEC values to crustaceans, mg/l	0.22 Daphnia (Calamari et al. 1982a)
LC50 values to fishes, mg/l	1.1 96hr, Salmo gairdneri (USEPA 1980b) 2.1 96hr, Pimephales (McCarty et al. 1985) 1.18 48hr, Salmo gairdneri 4.25 48hr, Brachydanio rerio (Calamari et al. 1983) 4.16 96hr, flow-through, Pimephales promelas 1.12 96hr, Salmo gairdneri (USEPA 1984)
EC50 values to fishes, mg/l	0.56–1.04 Pimephales promelas (Anon. 1986b) 1.1 96hr, Salmo gairdneri (USEPA 1984)
LOEC values to fishes, mg/l	0.76 Pimephales (USEPA 1980b)
NOEC values to fishes, mg/l	0.1 Salmo gairdneri, embryo (Calamari et al. 1982a) 0.565–1.04 32d, Pimephales promelas (USEPA 1984)

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Water solubility, mg/l	< 10 (MITI 1992)
Melting point, °C	133 (MITI 1992)
Log octanol/water coefficient, log Pow	3.56 (MITI 1992)
Total degradation in water	Biodegradation: 1% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	43–169 8w, Cyprinus carpio, conc 0.05 mg/l 78–213 8w, Cyprinus carpio, conc 0.005 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	1.8 48hr, Oryzias latipes (MITI 1992)

740 • 4,4'-Dichlorobenzilic acid ethyl ester 510-15-6

Sumformula of the chemical	C16H14C12O3
Water solubility, mg/l	> 20 (MITI 1992)
Melting point, °C	35–37 (MITI 1992)
Boiling point, °C	156–158 0.07 mmHg (MITI 1992)
Log octanol/water coefficient, log Pow	4.74 (MITI 1992)

Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	224–586 8w, Cyprinus carpio, conc 0.02 mg/l 256–709 8w, Cyprinus carpio, conc 0.002 mg/l (MITI 1992)
LC50 values to fishes, mg/l	1.94 48hr, Oryzias latipes (MITI 1992)

741 • 2,4-Dichlorobenzoic acid 50-84-0

Sumformula of the chemical	C7H4Cl2O2
EINECS-number	2000678
Water solubility, mg/l	600 (MITI 1992)
Melting point, °C	164 (MITI 1992)
Total degradation in water	Biodegradaation: 92% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).

742 • 2,6-Dichlorobenzoic acid 50-30-6

Water solubility, mg/l	16 (MITI 1992)
Melting point, °C	142–144 (MITI 1992)
Bioconcentration factor, fishes	< 0.2 6w, Cyprinus carpio, conc 1 mg/l < 1.8 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	> 1000 48hr, Oryzias latipes (MITI 1992)

743 • 3,4-Dichlorobenzoic acid 51-44-5

Water solubility, mg/l	42 (MITI 1992)
Melting point, °C	204–205 (MITI 1992)
Bioconcentration factor, fishes	< 0.2 6w, Cyprinus carpio, conc 1 mg/l < 2.3 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	182 48hr, Oryzias latipes (MITI 1992)

744 • 2,6-Dichlorobenzyl alcohol 15258-73-8

Water solubility, mg/l	1400 (MITI 1992)
Melting point, °C	98 (MITI 1992)
Log octanol/water coefficient, log Pow	1.98 (MITI 1992)
Bioconcentration factor, fishes	1.7–3.5 6w, Cyprinus carpio, conc 0.5 mg/l < 1.0–2.4 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	81.6 48hr, Oryzias latipes (MITI 1992)

745 • 3,4-Dichlorobenzyl alcohol 1805-32-9

Sumformula of the chemical	C7H6OCl2
Water solubility, mg/l	1600 (MITI 1992)
Melting point, °C	36–39 (MITI 1992)
Log octanol/water coefficient, log Pow	2.74 (MITI 1992)
Bioconcentration factor, fishes	1.7–3.5 6w, Cyprinus carpio, conc 0.05 mg/l < 2.8 6w, Cyprinus carpio, conc 0.005 mg/l (MITI 1992)
LC50 values to fishes, mg/l	8.98 48hr, Oryzias latipes (MITI 1992)

746 • 3,4-Dichlorobenzyl chloride 102-47-6

Water solubility, mg/l	20 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).

747 • 2,4'-Dichlorobiphenyl 34883-43-7

LC50 values to crustaceans, mg/l	0.12 96hr, Gammarus fasciatus (Mayer et al. 1977)

748 • 4,4'-Dichlorobiphenyl 2050-68-2

Molecular weight	223.1
Water solubility, mg/l	0.062 20 °C
Melting point, °C	142–145

Boiling point, °C	315–319	
Other information about degradation	32.4% degradation after 1hr by Alcaligenes Y42; 50.4% degradation after 1hr by Acinetobacter P6 at 11.1 mg/l initial concentration (Verschueren 1983).	
LC50 values to crustaceans, mg/l	0.1	96hr, Gammarus fasciatus (Mayer et al. 1977)

749 • 3,4-Dichlorobutene 64037-54-3 (rasemic mixture)

Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).

750 • 3,4-Dichlorocatechol 3978-67-4

LC50 values to algae, mg/l	0.3	96hr, Selenastrum capricornutum (Kuivasniemi et al. 1985)
LC50 values to fishes, mg/l	2.7	Oncorhynchus nerka (Durkin 1978)
	2.7	96hr, Salmo salar (Voss et al. 1980)

751 • 4,5-Dichlorocatechol 3428-24-8

LC50 values to algae, mg/l	0.4	96hr, Selenastrum capricornutum (Kuivasniemi et al. 1985)
LC50 values to fishes, mg/l	2.3	24hr, Salmo trutta (Hattula et al.1981)
	0.5–1.0	96hr, Salmo gairdneri (McKague 1981)

752 • Dichlorodehydroabietic acid 57055-39-7

LC50 values to fishes, mg/l	0.6	96hr, Salmo gairdneri (Leach & Thakore 1977)

753 • 1,1-Dichloroethane 75-34-3

Synonyms	Ethylidene chloride Ethylidene dichloride	
Sumformula of the chemical	C2H4Cl2	
Use	Intermediate.	
Molecular weight	98.96	
Water solubility, mg/l	5500	
Melting point, °C	-97	
Boiling point, °C	57.3	
Log octanol/water coefficient, log Pow	1.99	(Anon. 1988)
Henry's law constant, Pa x m³/mol	560 578.6	(Anon. 1988) calc. (Yaws et al. 1991)
Volatilization	Relative volatility (nBuAc=1) = 11.60	

Mobility	Equilibrium distribution:	
		mass %
	air	99.48
	water	0.52
	solid	0.00
		(Anon. 1988).
LD50 values to mammals in oral exposure, mg/kg	725	orl-rat (Lewis & Sweet 1984)
TDLo values to mammals in oral exposure, mg/kg	185	orl-mus (Lewis & Sweet 1984)
TCLo values to mammals in inhalation exposure, ppm	6000	ihl-rat, 6–15 d preg. (Lewis & Sweet 1984)
Maximum longterm immission concentration in air for plants,mg/m³	8	VDI 2306
Maximum longterm immission concentration in air for plants,ppm	2	VDI 2306
LC50 values to fishes, mg/l	550	96hr, Lepomis macrochirus
	480	96hr, Menidia audens
		(Dawson et al. 1977)
	200	7 d, Poecilia reticulata (Könemann 1979)

754 • 1,2-Dichloroethane 107-06-2

Synonyms	Ethane dichloride Ethylene dichloride Glycol dichloride	
Sumformula of the chemical	C2H4Cl2	
Use	Manufacturing of vinylchloride; manufacturing of etraethyllead; intermediate; insecticidal fumigant; ingredient in cosmetics; petrol additive.	
State and appearance	Colourless liquid.	
Odour	Quality: sweet Hedonic tone: unpleasant to neutral Threshold odour concentration absolute: 6.0 ppm 50% recognition: 40.0 ppm 100% recognition: 40.0 ppm Odour index 100% recognition: 2 037 (Hellman & Small 1974)	
Molecular weight	98.96	
Vapour pressure, mmHg	61	20 °C
Water solubility, mg/l	8690	20 °C
	8100	20 °C
	8800	25 °C (McConnell et al. 1975)
Melting point, °C	-35.36	(Suntio et al. 1988)
Boiling point, °C	83.5	
Log octanol/water coefficient, log Pow	1.45–1.79	(Sabljic 1987)
	2.82	(Anon. 1988)
	1.45	(Banerjee et al. 1980)
	1.48	(Hansch & Leo 1979

Henry's law constant, Pa x m³/mol	1000 1107.1 1125	(Anon. 1988) calc. (Dilling 1977) exptl. (Gossett 1987)
Volatilization	Evaporation from water (1 ppm, 25 °C): 50% after 29 min; 90% after 96 min (Verschueren 1983). Relative volatility (nBuAc=1) = 6.5	
Mobility	84.04% (air), 15.79% (water), 0.17% (sediment). Equilibrium distribution: air water solid	 *mass %* 99.97 0.03 0.00 (Anon. 1988).
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	670 489 860	orl-rat orl-mus orl-rbt (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	4886	skn-rbt (Lewis & Sweet 1984)
LC50 values to mammals in inhalation exposure, ppm	1000	432 min., ihl-rat (Verschueren 1983)
LDLo values to mammals in oral exposure, mg/kg	810 600 2000	orl-man (Lewis & Sweet 1984) orl-mus (Lewis & Sweet 1984) orl-dog (Lewis & Sweet 1984)
LDLo values to mammals in non-oral exposure, mg/kg	500 380 1200 600 175	scu-rat scu-mus scu-rbt ipr-gpg ivn-dog (Lewis & Sweet 1984)
LCLo values to mammals in inhalation exposure, mg/kg	5000	ihl-mus (Lewis & Sweet 1984)
LCLo values to mammals in inhalation exposure, ppm	3000	7hr, ihl-pig 7hr, ihl-rbt 7hr, ihl-gpg 4hr, ihl-rat (Lewis & Sweet 1984)
	3000	7hr, ihl-pig, 7hr, ihl-rbt 7hr, ihl-gpg 4hr, ihl-rat (Lewis & Sweet 1984)
	1500	7hr, ihl-pig 7hr, ihl-rbt 7hr, ihl-gpg 4hr, ihl-rat (Lewis & Sweet 1984)
	1000	7hr, ihl-pig 7hr, ihl-rbt 7hr, ihl-gpg 4hr, ihl-rat (Lewis & Sweet 1984)

TDLo values to mammals in oral exposure, mg/kg	38 orl-mus 18 orl-rat 428 orl-hmn (Lewis & Sweet 1984)
TDLo values to mammals in non-oral exposure, mg/kg	1120 skn-mus (Lewis & Sweet 1984)
TCLo values to mammals in inhalation exposure, ppm	4000 ihl-hmn (Lewis & Sweet 1984)
Carcinogenicity	NCI carcinogenesis bioassay completed: results positive; mus, rat (Lewis & Sweet 1984).
Maximum longterm immission concentration in air for plants,mg/m³	8 VDI 2306
Maximum longterm immission concentration in air for plants,ppm	2 VDI 2306
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 135 mg/l (Bringmann & Kühn 1980a)
EC50 values to microorganism, mg/l	1100 15 min Microtox (Hermens et al. 1985)
LOEC values to algae, mg/l	105 rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to crustaceans, mg/l	220 48hr, Daphnia magna (LeBlanc 1980) 65 96hr, Crangon crangon (Adema 1976) 268 48hr, unfed, Daphnia magna 315 48hr, fed, Daphnia magna (USEPA 1984)
EC50 values to crustaceans, mg/l	155 48hr, unfed, Daphnia magna 183 48hr, fed, Daphnia magna (USEPA 1984)
NOEC values to crustaceans, mg/l	10.6–20.7 28d, Daphnia (USEPA 1984)
LC50 values to fishes, mg/l	106 7 d, Poecilia reticulata (Könemann 1979) 118 96hr, Pimephales promelas (Veith et al. 1983) 430 96hr, Lepomis macrochirus (Buccafusco et al. 1981) 185 96hr, Gobius minutus (Adema 1976) 116 96hr, flow-through, Pimephales promelas (USEPA 1984)
LOEC values to fishes, mg/l	0.059 grw, schr, Pimephales promelas (Benoit et al. 1982)
NOEC values to fishes, mg/l	0.029 grw, schr, Pimephales promelas (Benoit et al. 1982) 29.0–59.0 32d, Pimephales promelas (USEPA 1984)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 710 mg/l protozoa (Entosiphon sulcatum): 1127 mg/l (Bringmann & Kühn 1980a)

755 • 1,1-Dichloroethylene 75-35-4

Synonyms	Vinylidene dichloride 1,1-Dichloroethene
Sumformula of the chemical	C2H2Cl2
Use	Adhesives; component of synthetic fibres; solvent

State and appearance	Colourless liquid.	
Molecular weight	96.94	
Vapour pressure, mmHg	500	20 °C
Water solubility, mg/l	200 980	20 °C (MITI 1992)
Melting point, °C	-122.5	(MITI 1992)
Boiling point, °C	31.7	(MITI 1992)
Log octanol/water coefficient, log Pow	2.17	(MITI 1992)
Henry's law constant, Pa x m³/mol	2316	calc. (Yaws et al. 1991)
Volatilization	Evaporation from water (1 ppm, 25 °C): 50% after 22 min; 90% after 89 min (Verschueren 1983).	
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 9.7 mg/l sludge: 2 mg/l (MITI 1992).	
Bioconcentration factor, fishes	2.5–6.4 < 13	6w, Cyprinus carpio, conc 0.5 mg/l 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
LD50 values to mammals in oral exposure, mg/kg	200	orl-rat (Lewis & Sweet 1984)
LC50 values to mammals in inhalation exposure, ppm	98	22hr, ihl-mus (Lewis & Sweet 1984)
LDLo values to mammals in oral exposure, mg/kg	5750	orl-dog (Lewis & Sweet 1984)
LDLo values to mammals in non-oral exposure, mg/kg	225 3700	ivn-dog scu-rbt (Lewis & Sweet 1984)
LCLo values to mammals in inhalation exposure, ppm	10000	24hr, ihl-rat (Lewis & Sweet 1984)
TDLo values to mammals in non-oral exposure, mg/kg	4840	skn-mus (Lewis & Sweet 1984)
TCLo values to mammals in inhalation exposure, ppm	25 55 55	ihl-hmn ihl-rat ihl-mus (Lewis & Sweet 1984)
Carcinogenicity	NTP carcinogenesis bioassay completed: results negative; mus, rat (Lewis & Sweet 1984).	
EC50 values to algae, mg/l	410	96hr, grw, Scenedesmus subspicatus (Geyer et al. 1985)
LC50 values to crustaceans, mg/l	79	48hr, Daphnia magna (LeBlanc 1980)

LC50 values to fishes, mg/l	74	96hr, Lepomis macrochirus (Buccafusco et al. 1981)
	220	96hr, Lepomis macrochirus
	250	96hr, Menidia audens (Dawson et al. 1977)
	108	96hr, Pimephales promelas (Dill et al. 1980)
	250	96hr, Cyprinodon variegatus (Heitmüller et al. 1981)
	220	96hr, Lepomis macrochirus (Dawson et al. 1977)
	> 20	48hr, Oryzias latipes (MITI 1992)

756 • 1,2-Dichloroethylene 540-59-0

Synonyms	Acetylene dichloride sym-Dichloroethylene	
Sumformula of the chemical	C2H2Cl2	
Use	Intermediate	
Molecular weight	96.94	
Log octanol/water coefficient, log Pow	2.55	(Anon. 1988)
Henry's law constant, Pa x m³/mol	3300	(Anon. 1988)
Mobility	Equilibrium distribution:	
		mass %
	air	99.91
	water	0.09
	solid	0.00
		(Anon. 1988).
LD50 values to mammals in oral exposure, mg/kg	770	orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	2000	ipr-mus (Lewis & Sweet 1984)
LC50 values to crustaceans, mg/l	220	48hr, Daphnia magna (LeBlanc 1980)
LC50 values to fishes, mg/l	140	96hr, Lepomis macrochirus (Buccafusco et al. 1981)

757 • cis-1,2-Dichloroethylene 156-59-2

Synonyms	cis-1,2-Dichloroethene	
Sumformula of the chemical	C2H2Cl2	
Use	Solvent.	
Molecular weight	96.94	
Water solubility, mg/l	5.6	(MITI 1992)
Melting point, °C	-80	(MITI 1992)
Boiling point, °C	60	(MITI 1992)
Log octanol/water coefficient, log Pow	1.83	(MITI 1992)

Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 2.62 mg/l sludge 2 mg/l 0% by BOD period: 28d substance: 6.43 mg/l sludge 2 mg/l (MITI 1992).
LCLo values to mammals in inhalation exposure, mg/kg	65000 2hr, ihl-mus 20000 6hr, ihl-cat (Lewis & Sweet 1984)

758 • trans-1,2-Dichloroethylene 156-60-5

Synonyms	trans-1,2-Dichloroethene	
Sumformula of the chemical	C2H2Cl2	
Use	Solvent.	
Molecular weight	96.94	
Water solubility, mg/l	4.1	(MITI 1992)
Melting point, °C	-50	(MITI 1992)
Boiling point, °C	48	(MITI 1992)
Log octanol/water coefficient, log Pow	1.92	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 2.32 mg/l sludge: 2 mg/l 0% by BOD period: 28d substance: 6.06 mg/l sludge: 2 mg/l (MITI 1992).	
LD50 values to mammals in non-oral exposure, mg/kg	7536 4019	ipr-rat ipr-mus (Lewis & Sweet 1984)
LCLo values to mammals in inhalation exposure, mg/kg	75000 43000	2hr, ihl-mus 6hr, ihl-cat (Lewis & Sweet 1984)
TCLo values to mammals in inhalation exposure, mg/kg	4800	10 min., ihl-hmn (Lewis & Sweet 1984)

759 • 4,5-Dichloroguaiacol 2460-49-3

Sumformula of the chemical	C7H6O2Cl2
Molecular weight	193
pKa	8.52

Log octanol/water coefficient, log Pow	3.23	(Xie 1984)
Mobility	1.62% (air), 77.05% (water), 21.33% (sediment)	
LC50 values to algae, mg/l	3.1	96hr, Selenastrum capricornutum (Kuivasniemi et al. 1985)
LC50 values to crustaceans, mg/l	3.1–6.2	Daphnia (Salkinoja-Salonen et al. 1981)
LC50 values to fishes, mg/l	2.3 4.8	96hr, Salmo gairdneri (Voss et al. 1980) Poecilia reticulata (Salkinoja-Salonen et al. 1981)

760 • 2,2'-Dichlorohydrazobenzene 782-74-1

Sumformula of the chemical	C12H10Cl2N2	
Water solubility, mg/l	< 10	(MITI 1992)
Melting point, °C	87	(MITI 1992)
Log octanol/water coefficient, log Pow	5.1	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	2650–5580 3140–5870	8w, Cyprinus carpio, conc 0.05 mg/l 8w, Cyprinus carpio. conc 0.005 mg/l (MITI 1992)
LC50 values to fishes, mg/l	62.1	48hr, Oryzias latipes (MITI 1992)

761 • Dichloroisopropyl ether 63283-80-7

Use	Solvent, byproduct.	
Molecular weight	171	
Log octanol/water coefficient, log Pow	2.5	(Anon. 1988)
Henry's law constant, Pa x m³/mol	11	(Anon. 1988)
Mobility	Equilibrium distribution: air water solid	*mass %* 78.49 20.51 0.99 (Anon. 1988).

762 • Dichloromethane 75-09-2

Synonyms	Methane dichloride Methylene chloride Methylene dichloride
Sumformula of the chemical	CH2Cl2

Use	Solvent. Aerosol propellant, paint remover, metal degreaser and a urethane foam blowing agent. (Chem. Mark. Report. 1983)
Molecular weight	84.93
Vapour pressure, mmHg	434.9 25 °C (Boublik et al. 1984)
Water solubility, mg/l	13200-20000 20 °C (Anon. 1986b) 13000 at 25 °C (Riddick et al. 1986) 7900 (MITI 1992)
Melting point, °C	-95.1 (Suntio et al. 1988)
Boiling point, °C	40 (Anon. 1986b) 38.5–40.5 (MITI 1992)
Log octanol/water coefficient, log Pow	1.25 (Anon. 1986b) 1.51 (Hansch & Leo 1979) 1.25 (Callahan et al. 1979) 1.25 (Hansch & Leo 1985) 1.25 (Sangster 1989)
Henry's law constant, Pa x m^3/mol	272 exptl. (Dilling 1977) 222 exptl. (Gossett 1987) 250.8 calc. (Yaws et al. 1991)
Volatilization	Relative volatility (nBuAc=1) = 27.5 Dichloromethane has a high Henry's Law coefficient and will evaporate rapidly from water. Half-lives for the evaporation from water of 3–5.6 hours have been determined at moderate mixing conditions. (Lyman et al. 1987) (Rathbun & Tai 1981) When dichloromethane released into an estuarine bay, all the chemical dissipated within 4 km of the release point in the spring and within 8 km in the winter under ice. (Howard II 1990) Due to high vapour pressure of dichloromethane, it will evaporate rapidly from near-surface soil. (Howard II 1990)
Mobility	log Kom 1.44 (Sabljic 1984) log Koc 1.68 (calc.) (Lyman et al. 1987) Dichloromethane is adsorbed strongly to peat moss, less strongly to clay, only slightly to dolomite limestone and not at all to sand. (Dilling et al. 1975)
Photochemical degradation in air	Since dichloromethane does not absorb light > 290 nm, it will not degrade by direct photolysis in the troposphere. (Hubrich & Stuhl 1980) Dichloromethane released into the atmosphere will degrade by reaction with hydroxyl radicals with a half-life of several months. A small fraction of the chemical will diffuse to the stratosphere where it will rapidly degrade by photolysis and reaction with chlorine radicals. (Howard II 1990)
Total degradation in water	Biodegradation: 5–26% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

Other information about degradation	Degradation of dichloromethane:

ENVIRONMENT	INIT.CONC. mg/l	REDOX-COND.	TEMP. °C	DEGRADATION %/day	REF.
water (adapted)	17	aerobic	30	100/0.5	a
water	17	anaerobic	30	60/0.5	a
water (deion.)	1	aerobic	25	t 1/2 = 540 d	b
water (adapted)	840	aerobic	-	100/0.75	c
water (adapted)	840	aerobic	-	80/30	c
water (abiotic)	-	-	25	t 1/2 = 700 yr	d
water (adapted)	5–10	aerobic	25	100/7	e
sandy soil	0.2	aerobic + natural gas		t 1/2 = 0.04 d	f

a) Brunner et al. 1980
b) Dilling et al. 1975
c) Kästner 1986
d) Schwarzenbach 1985
e) Tabak et al. 1981
f) Anon. 1987b
(Anon. 1987b).

Dichloromethane biodegrades completely under aerobic conditions with sewage seed or activated sludge between 6 hours to 7 days (Howard 1990).

86–92% conversion to C02 will occur after a varying acclimation period using anaerobic digestion in wastewater (Gossett 1985).

Bioconcentration factor, fishes	2.0–5.4	6w, Cyprinus carpio, conc 0.25 mg/l
	6.4–40	6w, Cyprinus carpio, conc 0.025 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	167	orl-rat (Lewis & Sweet 1984)
	3000	orl-dog (Anon. 1986b)
	2136	orl-rat (Anon. 1986b)
	1900	orl-rbt (Anon. 1986b)
LD50 values to mammals in non-oral exposure, mg/kg	1500	ipr-mus
	6460	scu-mus (Lewis & Sweet 1984)
LC50 values to mammals in inhalation exposure, mg/m³	88000	ihl-rat, 30 min.
	43400	ihl-cat, 4.5hr (Lewis & Sweet 1984)
LC50 values to mammals in inhalation exposure, ppm	14400	ihl-mus, 7hr
	14108	ihl-dog, 7hr
	5000	ihl-gpg, 2hr (Lewis & Sweet 1984)
LDLo values to mammals in oral exposure, mg/kg	3000	orl-dog
	1900	orl-rbt (Lewis & Sweet 1984)
LDLo values to mammals in non-oral exposure, mg/kg	950	ipr-dog
	2700	scu-dog
	200	ivn-dog
	2700	scu-rbt (Lewis & Sweet 1984)
TCLo values to mammals in inhalation exposure, ppm	500	ihl-hmn
	500	ihl-rat, 6hr (Lewis & Sweet 1984)
Maximum longterm immission concentration in air for plants,mg/m³	20	VDI 2306

Maximum longterm immission concentration in air for plants,ppm	5	VDI 2306
Effects on microorganisms	EC50 = 1000 mg/l, 15 min, Photobacterium phosphoreum EC50 = 2880 mg/l, 15 min, Photobacterium pho sphoreum (Anon. 1986b)	
EC50 values to microorganism, mg/l	2800	15 min Microtox (Hermens et al. 1985)
EC50 values to algae, mg/l	1000 662 662	24hr, assimilationtest 96hr, Selenastrum capricornutum chlorophyll a 96hr, Selenastrum capricornutum cellnumber (Anon. 1986b)
LC50 values to crustaceans, mg/l	220 224 220	48hr, Daphnia magna (LeBlanc 1980) 48hr, Daphnia magna (Anon. 1986b) 48hr, Daphnia magna (Anon. 1986b)
EC50 values to crustaceans, mg/l	2100	24hr, Daphnia magna (Anon. 1986b)
LC50 values to fishes, mg/l	193 294 330 220 502 471 528 521 193 310 224 220 331	96hr, Pimephales promelas (Alexander et al. 1978) 96hr, Poecilia reticulata (Könemann 1979) 96hr, Cyprinodon variegatus (Heitmuller et al. 1981) 96hr, Lepomis macrochirus (Buccafusco et al. 1981) 4d, Pimephales promelas 8d, Pimephales promelas (Dill et al. 1987) 48hr, 528/521 mg/l, Leuciscus idus melanotus 96hr, Pimephalis promelas 96hr, static, Pimephalis promelas 96hr, Lepomis macrochirus 96hr, Lepomis macrochirus (Anon. 1986b) 48hr, Oryzias latipes (MITI 1992)
EC50 values to fishes, mg/l	99	96hr, bhv, Pimephales promelas (Alecander et al. 1978)
Effects on the physiology of water organisms	Pimephales promelas, 82.5 mg/l, 28d, measurable change in length and/or weight (Dill et al. 1987).	
Other information about water organisms	50% pht inhibition = 1480 mg/l, Chlamydomonas angulosa, 50% pht inhibition = 2300 mg/l, Chlorella vulgaris, EC5 ≥ 8000 mg/l, 48hr, pH 6,9, Chilomonas paramaecium, EC5 ≥ 8000 mg/l, 72hr, pH 7, Entosiphon sulcatum EC5 ≥ 16000 mg/l, 20hr, pH 7, Uronema parduczi (Anon. 1986b)	

763 • Dichloromethyl benzene 98-87-3

Melting point, °C	-16	(MITI 1992)
Boiling point, °C	207	(MITI 1992)

Total degradation in water	Biodegradation: 89–92% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

764 • 4,5-Dichloronaphthalene-1,8-dicarboxylic acid

7267-11-0

Sumformula of the chemical	C12H6Cl2O4
Water solubility, mg/l	> 1000 (MITI 1992)
Bioconcentration factor, fishes	< 0.1–0.3 6w, Cyprinus carpio, conc 2 mg/l < 1.2–1.8 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 500 48hr, Oryzias latipes (MITI 1992)

765 • 4,4,5-Dichloronaphthalene-1,8-dicarboxylic anhydride

7267-14-3

Sumformula of the chemical	C12H4O3Cl2
Water solubility, mg/l	10 (MITI 1992)
Melting point, °C	> 300 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD (hydrolyzed to 4,5-Dichloronaphthalene-1,8-dicarbonylic acid) period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).

766 • 2,3-Dichloronitrobenzene

3209-22-1

EC50 values to microorganism, mg/l	1.3 Microtox (Kaiser and Ribo 1985)

767 • 2,4-Dichloronitrobenzene

611-06-3

EC50 values to microorganism, mg/l	3 Microtox (Kaiser and Ribo 1985)

768 • 2,5-Dichloronitrobenzene

89-61-2

EC50 values to microorganism, mg/l	7.8 Microtox (Kaiser and Ribo 1985)

769 • 3,5-Dichloronitrobenzene

618-62-2

EC50 values to microorganism, mg/l	22.6	Microtox (Kaiser and Ribo 1985)

770 • Dichlorophen

97-23-4

Synonyms	2,2'-Dihydroxy-5,5'-dichlorodiphenylmethane	
Use	Fungicide, bactericide, herbicide.	
Water solubility, mg/l	34	(MITI 1992)
Melting point, °C	177–178	(MITI 1992)
Log octanol/water coefficient, log Pow	4.96	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	26–84 98–281	8w, Cyprinus carpio, conc. 0.05 mg/l 8w, Cyprinus carpio, conc 0.005 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	3.6 5.4 1.35	96hr, Rasbora heteromorpha 24hr, Rasbora heteromorpha (Tooby et al. 1975) 48hr, Oryzias latipes (MITI 1992)

771 • 2,3-Dichlorophenol

576-24-9

Sumformula of the chemical	C6H4OCl2	
Molecular weight	163	
Water solubility, mg/l	3600	(MITI 1992)
Melting point, °C	57	(MITI 1992)
pKa	7.71	(Doedens 1967)
Log octanol/water coefficient, log Pow	3.15 2.95	(Banerjee et al. 1984) (MITI 1992)
Log soil sorption coefficient, log Kom	2.65 2.77	observed (Sabljic 1987) calculated (Sabljic 1987)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	7.4–35 6.7–20	6w, Cyprinus carpio, conc 0.03 mg/l 6w, Cyprinus carpio, conc 0.003 mg/l (MITI 1992)

Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	6 48hr, Oryzias latipes (MITI 1992)

772 • 2,4-Dichlorophenol 120-83-2

Sumformula of the chemical	C6H4OCl2
Use	Organic synthesis.
Molecular weight	163
Water solubility, mg/l	4600 20 °C 4500 20 °C, pH 5.1 (Blackman et al. 1955) 4670 25 °C (Cheung 1984) 2400 (MITI 1992)
Melting point,°C	45 (MITI 1992)
Boiling point, °C	210 (MITI 1992)
pKa	7.68 (Doedens 1967)
Log octanol/water coefficient, log Pow	2.80–3.23 (Sabljic 1987) 2.75 observed (Chin et al. 1986) 3.22 (Xie 1984) 3.3 (Hansch & Leo 1979) 3.06 (Hansch & Leo 1979) 3.08 (Hansch & Leo 1979) 3.15 (MITI 1992)
Log soil sorption coefficient, log Kom	2.75 observed (Sabljic 1987) 2.76 calculated (Sabljic 1987)
Henry's law constant, Pa x m^3/mol	0.4044 calc. (Suntio et al. 1988)
Aerobic degradation in soil	AEROBIC DEGRADATION IN SOIL Maximum adsorption wavelength: 286 nm NON-STERILE SOIL Minimum time for > 70% decrease: 7.00–20.00 d % decomposition at the termination of the experiment: 40d, 81% STERILE SOIL % decomposition at the termination of the experiment: 40d, 31% (Baker et al. 1980)
Anaerobic degradation in soil	ANAEROBIC DEGRADATION IN SOIL Maximum adsorption wavelength: 286 nm NON-STERILE SOIL % decomposition at the termination of the experiment: 80d, 62% STERILE SOIL % decomposition at the termination of the experiment: 80d, 59% (Baker et al. 1980)
Total degradation in soil	Decomposition rate in soil: 9 days for complete disappearance (Verschueren 1983).
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

Bioconcentration factor, fishes	34	Carassius auratus
	7.1–69	8w, Cyprinus carpio, conc 0.03 mg/l
	13–55	8w, Cyprinus carpio, conc 0.003 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	580	orl-rat
	464	orl-mam (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	790	skn-mam (Lewis & Sweet 1984)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 6 mg/l (Bringmann & Kühn 1980a)	
EC50 values to microorganism, mg/l	49.5	OECD 209 (Klecka et al. 1985)
LOEC values to algae, mg/l	2	rpd, schr, Microcystis aeruginosa (Pitter 1976)
LC50 values to crustaceans, mg/l	2.6	48hr, Daphnia magna (LeBlanc 1980)
LC50 values to fishes, mg/l	0.08	23 days, Salmo gairdneri (embryo)
	0.08	96hr, Salmo gairdneri(larva) (Birge et al. 1979)
	2.8	96hr, Salmo gairdneri (Voss et al. 1980)
	2.6	96hr, Salmo gairdneri (Hodson et al. 1984)
	4.2	24hr, Poecilia reticulata (Könemann 1979)
	3.9	96hr, Branchydanio rerio,
	5	48hr, Leuciscus idus (Wellens 1982)
	8.6	48hr, Oryzias latipes (MITI 1992)
LOEC values to fishes, mg/l	0.46	srv, schr, Pimephales promelas (Holcombe et al. 1982)
Other information about water organisms	LOEC 0.5 mg/l, rpd, schr, Entosiphon sulcatum (Bringmann & Kühn1980a). EC50 15.0 mg/l, grw, 2 d, Tetrahymena pyriformis (Schultz 1987). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 3.6 mg/l protozoa (Entosiphon sulcatum): 0.5 mg/l (Bringmann & Kühn 1980a)	

773 • 2,5-Dichlorophenol 583-78-8

Synonyms	2,5-DCP	
Sumformula of the chemical	C6H4Cl2O	
Odour	Odour threshold, water: 0.00045–0.0033 mg/l; 0.033 mg/l at 30 °C; 0.030 at 20–22 °C (Sax 1986). Taste threshold: 0.0005 mg/l in water; the 48hr threshold taste impairment limit for rainbow trout is 0.023 mg/l (Sax 1986).	
Molecular weight	163.01	
Water solubility, mg/l	> 2000	(MITI 1992)

D

Melting point, °C	58 (MITI 1992)
Boiling point, °C	211 744 mmHg (MITI 1992)
pKa	0.00000045 0.000000031 0.000000045
Log octanol/water coefficient, log Pow	3.2 (Sax 1986) 3.23 (MITI 1992)
Adsorption/desorption	Sorption of 2,5-DCP by Bentone 24 (Wyoming bentonite coated with dimethylbenzyl octadecylammonium chloride), an organo-clay, was studied. Sorption was accomplished from solution at 20 °C, during 45 to 48 hours constant shaking period in darkened rooms. The 2,5-DCP concentration was 0.5 mM with 5 g Bentone 24 in a 0.005 M KHCO3 buffer. Solutions at pH 7.9 (pKa = 7.35, 76% protolysis) and 7.5 (59% protolysis) were studied. At pH 7.9, 93.9% of the initial amount was sorbed, and at pH 7.5, 38% of the initial amount was sorbed onto the bentone 18C (a Wyoming bentonite with sorbed dodecylamine) under similar conditions (Sax 1986).
Other physicochemical properties	Sparingly soluble in water (Sax 1986).
Total degradation in soil	Microbial decomposition in soils was studied using the shake culture method. The medium was composed of the following: 0.5 g ammonium nitrate, 0.2 g monobasic and 0.8 g dibasic potassium phosphate, 0.2 g magnesium sulfate, 0.03 g ferrous sulfate and 0.1 g calcium chloride in 1000 ml of distilled H2O. The medium was sterilized and had a pH of 7.2. 2,5-DCP was added to a final concentration of 0.050 mg per ml and 4 g of freshly sampled Dunkirk silt loam soil was added to 100 ml of the medium as an inoculum. Temperature was 30 °C and cultures were aerated on the shaker. UV spectrophotometry was to measure persistence. Days for complete disappearance was not attained due to its persistence for the duration of the incubation (72 days). – Biological degradation in activated sludge showed 52 % ring degradation in four days from an initial concentration of 100 mg/l. The sludge was acclimated, pH 7.0, 26 °C and UV spectrophotometry was the method of analysis (Sax 1986).
Total degradation in water	Biodegradation: 5% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	4.0–35 6w, Cyprinus carpio, conc 0.03 mg/l 4.8–16 6w, Cyprinus carpio, conc 0.003 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon.1987).
LC50 values to fishes, mg/l	1.7 96hr, Salmo salar (Voss et al. 1980) 2.7 24hr, Poecilia reticulata (Könemann 1979) 4.2 48hr, Oryzias latipes (MITI 1992)

774 • 2,6-Dichlorophenol 87-65-0

Synonyms	2,6-DCP
Sumformula of the chemical	C6H4Cl2O
Odour	Odour threshold, water: 0.003 mg/l at 30 °C; 0.200 mg/l at 20–22 °C; taste threshold: 0.002 mg/l; 0.0002 mg/l; 48hr treshold limits for impairment of taste in rainbow trout is 0.035 mg/l (Sax 1986).
Molecular weight	163

Vapour pressure, mmHg	1 59.5 °C
Water solubility, mg/l	1900 (MITI 1992)
Melting point, °C	68–69 °C (Suntio et al. 1988) 67 (MITI 1992)
Boiling point, °C	219–220 (MITI 1992)
pKa	0.00000016, 25 °C 0.0000002 6.8 (Doendens 1967)
Log octanol/water coefficient, log Pow	2.57 (Sax 1986) 2.88 (Xie 1984) 2.84 (Hansch & Leo 1979) 3.33 (Banerjee et al. 1984) 2.98 (MITI 1992)
Adsorption/desorption	Sorption of 2,6-DCP by Bentone 24 (Wyoming bentonite coated with dimethyl-benzyl octadecylammonium chloride), an organo-clay, was studied. Sorption was accomplished from solution at 20° during 45 to 48hr constant shaking period in darkened rooms. The 2,6-DCP concentration was 0.5 mM with 5 g Bentone 24 in a 0.005 M KHCO3 buffer. Solutions examined had PHs of 7.8 (pKa 6.8, 91% protolysis) and 7.4 (82% protolysis). Analysis was via UV-technique. At pH 7.8, 78.6 or the initial amount was sorbed, and at pH 7.4, 32% of the initial amount was sorbed onto Bentone 13C (a Wyoming Bentonite with one symmetry of sorbed dodecylamine (Sax 1986).
Aerobic degradation in soil	AEROBIC DEGRADATION IN SOIL Maximum adsorption wavelength: 284 nm NON-STERILE SOIL Minimum time for > 70% decrease: 0.25–0.50 d % decomposition at the termination of the experiment:0.75d, 100% STERILE SOIL % decomposition at the termination of the experiment: 40d, 55% (Baker et al. 1980)
Anaerobic degradation in soil	ANAEROBIC DEGRADATION IN SOIL Maximum adsorption wavelength: 284 nm NON-STERILE SOIL Minimum time for > 70% decrease: 10.00–24.00 d % decomposition at the termination of the experiment: 80d, 82% STERILE SOIL Minimum time for > 70% decrease: 24.00–80.00 d % decomposition at the termination of the experiment: 80d, 81% (Baker et al. 1980)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	4.1–20 6w, Cyprinus carpio, conc 0.03 mg/l 6.5–15 6w, Cyprinus carpio (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	2940 orl-rat (Sax 1986)

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LD50 values to mammals in non-oral exposure, mg/kg	390 ipr-rat 1730 scu-rat (Sax 1986)
Effects on the physiology of mammals	The inhibition of oxidative phosphorylation by 50% was shown at a concentration of 0.00000400 M in rat liver mitochondria. Measurement was via oxygen consumption using polarographic techniques (Sax 1986).
Health effects	500 mg applied to rabbit skin for 24 hours caused severe irritation (Sax 1986). Poisoned rats suffered convulsions and slight hypothermia (Sax 1986). Skin and eye irritation data: skn, rbt, 500 mg, 24hr, severe; eye, rbt, 0.250 mg, 24hr, severe (Sax 1986).
Mutagenicity	2,6-dichlorophenol was not mutagenic according to the salmonella-mammalian microsome ames assay. Both activated and unactivated systems were used (Sax 1986).
Effects on wastewater treatment	Phenol may be converted to 2,6-dichlorophenol during the chlorination reactions of the water treatment process (Sax 1986).
EC50 values to algae, mg/l	9.7 96hr, Chlorella vulgaris, grw 29 96hr, Selenastrum capricornutum, grw (Shigeoka et al. 1988)
LC50 values to crustaceans, mg/l	12.225 Daphnia magna, 7d (LeBlanc et al. 1988)
EC50 values to crustaceans, mg/l	3.83–5.151 7d, Daphnia magna enzyme effect (LeBlanc et al. 1988)
LC50 values to fishes, mg/l	4 48hr, Leuciscus idus (Dietz & Traud 1978) 11.3 48hr, Oryzias latipes (MITI 1992)
Other information about water organisms	Crangon septemspinosa, 52hr, effect level, 19.1 mg/l (Sax 1986).

775 • 3,4-Dichlorophenol 95-77-2

Water solubility, mg/l	> 1000 (MITI 1992)
Melting point, °C	68 (MITI 1992)
Boiling point, °C	253.5 (MITI 1992)
Log octanol/water coefficient, log Pow	3.21 (MITI 1992)
Aerobic degradation in soil	AEROBIC DEGRADATION IN SOIL Maximum adsorption wavelength: 285 nm NON-STERILE SOIL Minimum time for > 70% decrease: 80.0–160.0 d % decomposition at the termination of the experiment: 160d, 88% STERILE SOIL % decomposition at the termination of the experiment: 160d, 21% (Baker et al. 1980).
Anaerobic degradation in soil	ANAEROBIC DEGRADATION IN SOIL Maximum adsorption wavelength: 285 nm NON-STERILE SOIL % decomposition at the termination of the experiment: 160d, -4% STERILE SOIL % decomposition at the termination of the experiment: 160d, -3% (Baker et al. 1980).

Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	22–84 16–82	8w, Cyprinus carpio, conc 0.03 mg/l 8w, Cyprinus carpio, conc 0.003 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
EC50 values to microorganism, mg/l	74	INT (Dutton et al. 1986)
LC50 values to fishes, mg/l	2.6	48hr, Oryzias latipes (MITI 1992)

776 • 3,5-Dichlorophenol

591-35-5

Water solubility, mg/l	> 1000	(MITI 1992)
Melting point, °C	68	(MITI 1992)
Boiling point, °C	233–234	(MITI 1992)
Log octanol/water coefficient, log Pow	3.43	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	9.1–82 12–152	8w, Cyprinus carpio, conc 0.03 mg/l 8w, Cyprinus carpio, conc 0.003 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
EC50 values to microorganism, mg/l	6-22 4.5 10.1 12.5	3hr Act. sludge respiration (King and Painter 1986) Microtox (Reteuna et al. 1986) 3hr Act. sludge respiration (Reteuna et al. 1986) OECD 209 (Klecka et al. 1985)
LC50 values to fishes, mg/l	2.95	48hr, Oryzias latipes (MITI 1992)

777 • 3-(3,4-Dichlorophenyl)-1-methyl-1-n-butylurea

555-37-3

Synonyms	Dichlorophenyl methyl butylurea	
Use	Pesticide.	
EC50 values to algae, mg/l	0.02	10 days, pht, Chlorococcum sp., Dunaliella terticulata (Walsh 1972)

778 • N-(3,4-Dichlorophenyl)-N'-(2'-(4"-chloro-2"-sulfophenoxy)-5'-chlorophenyl)urea 24019-05-4

Sumformula of the chemical	C19H12O5N2SCl4
Water solubility, mg/l	800 (MITI 1992)
Melting point, °C	145–160 (MITI 1992)
Log octanol/water coefficient, log Pow	1.55 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	21–74 6w, Cyprinus carpio, conc 0.2 mg/l 33–114 6w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
LC50 values to fishes, mg/l	26 48hr, Oryzias latipes (MITI 1992)

779 • 2,4-Dichlorophenyl p-nitrophenyl ether 1836-75-5

Synonyms	2,4-Dichloro-4'–nitrodiphenyl ether 2,4-Dichloro-1-(4-nitrophenoxy)benzene 2,4-Dichlorophenylp-nitrophenyl ether 2,4-Dichlorophenyl 4-nitrophenyl ether Nitrofen Nitrophen Nitrophene
Sumformula of the chemical	C12H7Cl2NO3
Use	Herbicide.
Molecular weight	284.1
LD50 values to mammals in oral exposure, mg/kg	740 orl-rat 450 orl-mus 1620 orl-rbt (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	5000 skn-rat 3000 unk-rat (Lewis & Sweet 1984)
LDLo values to mammals in oral exposure, mg/kg	300 orl-cat (Lewis & Sweet 1984)
LCLo values to mammals in inhalation exposure, mg/kg	620 4hr, ihl-cat (Lewis & Sweet 1984)
TDLo values to mammals in oral exposure, mg/kg	180 orl-rat 42 7-15 days pregnant 114 orl-rat orl-mus (Lewis & Sweet 1984)

Carcinogenicity	NCI carcinogenesis bioassay completed; results positive; mouse, rat (NCITR NXI-CG-TR-22,78) (Lewis & Sweet 1984). NCI carcinogenesis bioassay completed; results positive; mouse (NCITR NXI-CG-TR-184,79) (Lewis & Sweet 1984). NCI carcinogenesis bioassay completed; results negative; rat (NCITR NXI-CG-TR-184,79 (Lewis & Sweet 1984).
Effects on plants	Application of nitrofen with a sprayer at 1.12 kg/ha caused damage to sainfoin seedlings (Onobrychis viciaefolia) grown in the greenhouse (Waddington 1978).
LC50 values to crustaceans	> 40 act, Daphnia pulex (Hashimoto & Nishiuchi 1981)
LC50 values to fishes, mg/l	1.59 96hr, Poecilia reticulata (Kam-Wing & Furtado 1978) 2.1 48hr, Cyprinus carpio 1.4 48hr, Carassius auratus (Hashimoto & Nishiuchi 1981)

780 • Dichlorophenylphosphine 644-97-3

Sumformula of the chemical	C6H5C12P
Melting point, °C	-51 (MITI 1992)
Boiling point, °C	222 759 mmHg (MITI 1992)
Total degradation in water	Biodegradation: 0–16% by BOD (hydrolyzed to Phenylphosphinic acid) period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

781 • 3,6-Dichloropicolinic acid 1702-17-6

Synonyms	Clopyralid Matrigon * 3,6-Dichloropyridine-2-carboxylic acid Dowco 290 Lontrel 100 *
Sumformula of the chemical	C6H3Cl2NO2
Products containing the chemical	Matrigon * clopyralid 100 g/l (PESREG) Lontrel * clopyralid 100g/l (PESREG)
Use	Active ingredient in herbicides.
State and appearance	Colourless crystals.
Molecular weight	192
Vapour pressure, mmHg	0.000012 25 °C (PESREG)
Water solubility, mg/l	9000 20 °C (Pesticide Manual 1987) 10000 pH 2.3, 24 °C (PESREG)
Melting point, °C	151–152 (PESREG)
pKa	2.33(PESREG)
Log octanol/water coefficient, log Pow	-0.198 at 21 °C, Test A8 84/449/EEC, GLP (PESREG)
Log air/water coefficient, log Paw	6.98 (PESREG)

Log soil sorption coefficient, log Kom	0.3 (Sabljic 1987) 1 (PESREG)
Mobility	The leaching behaviour of clopyralid (300 g a.i./ha) was studied in the field with two soils (rainfall 231 mm and 133.5 mm).12 weeks after application clopyralid residue level in the 0–15 cm soil samples were from 0.03 to 0.01 ppm (PESREG). The leaching behaviour of clopyralid (200 g and 400 g a.i./ha) was studied in the sandy loam soil.

applic. rate g a.i./ha	*depth inch.*	*clopyralid 44 days*	*residue ppb 150 days*
200	0–6	17.1	1.1
	6–12	12.7	
	12–18	1.6	
400	0–6	33.4	15.4
	6–12	4.0	9.8

(PESREG)

Other physicochemical properties	Solubility in organic solvents (g/100 ml) at 20 °C acetone: > 25 xylene: > 25 cyclohexanone: > 25 methanol: > 25 (PESREG).
Photochemical degradation in water	The photolysis and hydrolysis rates of clopyralid in buffered distilled water and in natural water were studied for the pH range 4.7 to 8.1. There is virtually no decomposition over 30 days of continuous exposure to light. There was a small amount (2.5%) of decomposition at pH 6.9 and under the 60 days. The decomposition product was 3-chloro-6-hydroxy-picolinic acid (PESREG).
Hydrolysis in water	The hydrolysis of clopyralid was studied at 25 °C in the dark, in sterile, buffered water at pH 5, 7 and 9. No hydrolytic dacay of clopyralid was observed at the pH values over a 30-day time period (GLP) (PESREG).
Aerobic degradation in soil	The degradation rate of clopyralid was studied in two different soils. The soils were incubated at three temperatures, at five moisture levels and at two concentrations.

*half-life * days*	*temperature °C*	*moisture ** %*	*concentration ppm*
202	15	100	0.25
36	25	100	0.25
21	35	100	0.25
316	25	air dry	0.25
85	25	32	0.25
36	25	50	0.25
35	25	75	0.25
120	25	100	1.00

* average half-life values from the soils
** the moisture content of field capacity

14CO2 amount increased from 27% to 67% after 200 days, when the temperature increased from 15 °C to 25 °C. 14CO2 amount increased from 0.14% to 60% after 100 days, when the moisture increased from air dry to 75% of field capacity (PESREG).

The decomposition of clopyralid was studied under aerobic conditions in two sterile and non-sterile soils at 25 °C and moisture content 75%. The half-lives were 62 days (loam soil) and 12 days (silty clay loam) in non-sterile conditions. No apparent decomposition was observed in sterile soil after 100 days incubation (PESREG).

	The half-lives of clopyralid were studied under aerobic conditions in ten different soils. The half-lives were from 15 days to 278 days, in eight cases they were < 48 days (PESREG).	
Other information about degradation	The degradation of clopyralid was studied in two soils under three different conditions: aerobic, aerobic (30 days/water- logged (270 days) and waterlogged (300 days). In aerobic conditions the half-life was from 12 to 31 days. Under aerobic/waterlogged conditions there was appr. 1% of the applied radioactivity present as clopyralid after 300 days incubation. Under complete waterlogged conditions there was appr. 22% of applied clopyralid was degraded after 300 days of incubation (PESREG).	
Bioconcentration factor, fishes	< 1, 1 ppm, 28d+14d, Lepomis macrochirus (PESREG)	
LD50 values to mammals in oral exposure, mg/kg	5000 1621 > 5000	orl-rat (PESREG) orl-rbt (PESREG) Matrigon (PESREG)
LD50 values to mammals in non-oral exposure, mg/kg	> 2000 > 2000 > 2000	idr-rat (Matrigon *) (PESREG)) idr-rat (PESREG) idr-rbt (PESREG)
LC50 values to mammals in inhalation exposure, mg/m³	> 1300	mg/m³, 4hr, ihl-rat (PESREG)
LD50 values to birds in oral exposure, mg/kg	1465	orl-Anas platyrhynchos (PESREG)
Subacute LC50 values to birds in feeding exposure, mg/kg	> 4640 > 4640	8d, Anas platyrhynchos 8d, Coturnix virginianus (PESREG)
Effects on invertebrates	LC50, > 1000 mg/kg, 14d, Eisenia foetida A 9.8% reduction in bodyweight at 1000 mg/kg level after 14 days exposure. GLP, OECD (PESREG)	
Effects on bees	LD50, > 0.1 mg/bee, 48hr, oral and contact, at 25 °C (PESREG)	
Effects on microorganisms	Clopyralid treatment (1 and 10 ppm) didn't cause any significant effect on the nitrification process, nitrogen fixing microbes or the degradation of carbonaceous materials by soil (five different soils) microbes. (PESREG)	
EC50 values to algae, mg/l	730 449	72 hr, ErC50, grw ihb, Selenastrum capricornutum, Lontrel 100 * 72 hr, EbC50, grw ihb, Selenastrum capricornutum, Lontrel 100 * EPA, OECD No 201 (PESREG)
LC50 values to crustaceans, mg/l	779.5 217.8	48 hr, Daphnia magna 20d, semi-static, Daphnia magna Lontrel 100 *, GLP, OECD No 202 (PESREG)
	1228.5	48 hr, Daphnia magna, Lontrel 100 * GLP, OECD No 202 (PESREG)
	232 241	48 hr, Daphnia magna, GLP (PESREG) 48 hr, Daphnia magna, GLP (PESREG)
EC50 values to crustaceans, mg/l	205.9	20d, rpd, semi-static, Daphnia magna Lontrel 100 *, GLP, OECD No 202 (PESREG)

LC50 values to fishes, mg/l	103.5 125.4	96 hr, Salmo gairdneri 96 hr, Lepomis macrochirus (Pesticide Manual 1983)
	500	96 hr, Salmo gairdneri, Lontrel 100 * GLP, OECD No 203 (PESREG)
	321.1	21d, semi-static, Salmo gairdneri Lontrel 100 *, GLP, OECD No 204 (PESREG)
	103.5 125.4	96 hr, Salmo gairdneri (PESREG) 96 hr, Lepomis macrochirus (PESREG)
LOEC values to fishes, mg/l	500	96hr, Salmo gairdneri, Lontrel 100 * GLP, OECD No 203 (PESREG)
NOEC values to fishes, mg/l	250	96hr, Salmo gairdneri, Lontrel 100 * GLP, OECD No 203 (PESREG)
	125	21d, semi-static, Salmo gairdneri Lontrel 100 *, GLP, OECD No 204 (PESREG)

D

782 • Dichloropropane 26638-19-7

Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).

783 • 1,1-Dichloropropane 78-99-9

LC50 values to crustaceans, mg/l	23	48hr, Daphnia magna (LeBlanc 1980)
LC50 values to fishes, mg/l	98	96hr, Lepomis macrochirus (Buccafusco et al. 1981)

784 • 1,2-Dichloropropane 78-87-5

Synonyms	Propylene dichloride	
Use	Solvent; Intermediate.	
Odour	Quality: sweet Hedonic tone: pleasant Threshold odour concentration absolute: 0.25 ppm 50% recognition: 0.50 ppm 100% recognition: 0.60 ppm Odour index 100% recognition: 87 096 (Hellman & Small 1974)	
Molecular weight	113	
Water solubility, mg/l	> 1000	(MITI 1992)
Boiling point, °C	96.4	(MITI 1992)
Log octanol/water coefficient, log Pow	2.24	(Anon. 1988)
Henry's law constant, Pa x m^3/mol	280 271	(Anon. 1988) calc. (Yaws et al. 1991)

Mobility	Equilibrium distribution: *mass %* air 98.95 water 1.02 solid 0.02 (Anon. 1988).	
Half-life in soil, days	55	(Li et al. 1990)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	1.2–3.2 0.5–6.9	6w, Cyprinus carpio, conc 0.4 mg/l 6w, Cyprinus carpio, conc 0.04 mg/l (MITI 1992)
LD50 values to mammals in oral exposure, mg/kg	1900	orl-rat
LC50 values to crustaceans, mg/l	52	48hr, Daphnia magna (LeBlanc 1980)
LC50 values to fishes, mg/l	320 240	96hr, Lepomis macrochirus 96hr, Menidia audens (Dawson et al. 1977)
	280	96hr, Lepomis macrochirus (Buccafusco et al. 1981)
	140	96hr, Pimephales promelas (Broderius & Kahl 1985)
	140	96hr, flow-through, Pimephales promelas (USEPA 1984)
	104	48hr, Oryzias latipes (MITI 1992)
LOEC values to fishes, mg/l	0.011	grw, schr, Pimephales promelas (Benoit et al. 1982)
NOEC values to fishes, mg/l	0.006	grw, schr, Pimephales promelas (Benoit et al. 1982)
	6.0–11.0	32d, Pimephales promelas (USEPA 1984)

785 • 1,3-Dichloropropane 142-28-9

Henry's law constant, Pa x m³/mol	100.5	calc. (Yaws et al. 1991)
LC50 values to fishes, mg/l	160	24hr, Carassius auratus (Bridie et al. 1979)
	131	96hr, flow-through, Pimephales promelas (USEPA 1984)
NOEC values to fishes, mg/l	8.0–16.0	32d, Pimephales promelas (USEPA 1984)

786 • 1,3-Dichloropropene 542-75-6

Synonyms	1,3-Dichloro-1-propylene	
State and appearance	Clear light straw coloured liquid.	
Molecular weight	110.97	
Vapour pressure, mmHg	43 34	25 °C (cis) 25 °C (trans)
Water solubility, mg/l	2700 2800	(cis) (trans)

Boiling point, °C	104 112	(cis) (trans)
Volatilization	Evaporation from water (1 ppm, 25 °C): 50% after 31 min; 90% after 98 min (Verschueren 1983).	
Chemical oxygen demand, g 02/g	0.84	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.19	5 days (Bridie et al. 1979)
LD50 values to mammals in oral exposure, mg/kg	250	orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	504	skn-rbt (Lewis & Sweet 1984)
LC50 values to crustaceans, mg/l	6.2	48hr, Daphnia (LeBlanc 1980)
LC50 values to fishes, mg/l	3.94 1.8 7.09 6.1	96hr, Salmo gairdneri (Pesticide Manual 1983) 96hr, Cyprinodon variegatus (Heitmuller et al. 1981) 96hr, Lepomis macrochirus (Pesticide Manual 1983) 96hr, Lepomis macrochirus (Buccafusco et al. 1981)

787 • 2,3-Dichloropropene 78-88-6

LC50 values to fishes, mg/l	1.1	14 d, Poecilia reticulata (Hermens et al. 1985)

788 • 2,2-Dichloropropionic acid, sodium salt 127-20-8

Synonyms	DPA Dalapon Dalapon sodium α,α-Dichloropropionic acid sodium salt Dowpon Sodium α,α-dichloropropionate Sodium 2,2-dichloropropionate	
Sumformula of the chemical	C3H3Cl2O2Na	
Use	Herbicide.	
Molecular weight	164.95	
Water solubility, mg/l	500000 soluble	25 °C (MITI 1992)
Melting point, °C	214	(MITI 1992)
Total degradation in soil	75–100% disappearance from soils: 8 weeks (Verschueren 1983).	
Total degradation in water	Biodegradation: 13.7% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	0.49–1.5 < 0.32–14	6w, Cyprinus carpio, conc 3 mg/l 6w, Cyprinus carpio, conc 0.3 mg/l (MITI 1992)

Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	4500 3860 3400 40000	orl-rbt orl-rat (Lewis & Sweet 1984) orl-gpg orl-mam (Sweet 1987)
Mutagenicity	Mutation data: Cytogenic analysis; mouse, unreported route, 200 mg/kg (Sweet 1987).	
LD50 values to birds in oral exposure, mg/kg	5600	orl-ckn (Lewis & Sweet 1984)
Effects on plants	2.8 kg dalapon/ha a.e. was applied to ryegrass populations (Lolium perenne) → yield reductions (Charles et al. 1978) Incubation of segments of barley col optile and Sesbania exaltata hypocotyls in 1% sucrose containing 2 ppm dalapon inhibited protein synthesis by 7 and 4%, respectively (Mann et al. 1965) Germinated seedlings of barley (Hordeum vulgare) were grown in dalapon-treated silica sand: 650 ppm dalapon (in mg active material per litre solution; 12 ml of the solution was added to 225 g dry sand) caused 70% reduction in barley root growth (O'Sullivan & Prendeville 1974)	
EC50 values to algae, mg/l	20	10 d, Chlorococcum sp. etc. Dunaliella terticulata Phaeodactylum tricornutum (Walsh 1972)
LC50 values to crustaceans, mg/l	6 16 11 1505	48hr, Daphnia magna (F.W.P.C.A. 1968) 48hr, Simocephalus serrulatis 48hr, Daphnia pulex (Sanders & Cope 1966) act, Daphnia magna (Kenaga 1979)
LC50 values to fishes, mg/l	> 87 290 340 115 223 < 100 350 650	Salmo gairdneri (Kenaga 1979) 96hr, Pimephales promelas Poecilia reticulata (Surber & Pickering 1962) 48hr, Oncorhynchus kisutch (Bond et al. 1960) 96hr, Lepomis macrochirus (Edwards 1977) 96hr, Poecilia reticulata (Kam Wing & Furtado 1977) act, Lepomis macrochirus 24hr, Salmo gairdneri (Alabaster 1969) 48hr, Oryzias latipes (MITI 1992)

789 • 2,6-Dichloropyridine

2402-78-0

Sumformula of the chemical	$C_5H_3Cl_2N$	
EC50 values to microorganism, mg/l	80.8	Microtox (Kaiser and Ribo 1985)

790 • 9,10-Dichlorostearic acid

5829-48-1

LC50 values to fishes, mg/l	1.5	96hr, Salmo gairdneri (Leach & Thakore 1975)

791 • 2,4-Dichlorotoluene 95-73-8

LC50 values to fishes, mg/l	4.6	14 d, Poecilia reticulata (Könemann 1979)

792 • 3,4-Dichlorotoluene 95-75-0

EC50 values to microorganism, mg/l	1.4	15 min Microtox (Hermens et al. 1985)
LC50 values to fishes, mg/l	5 2.91	7 d, Poecilia reticulata (Könemann 1979) 96hr, Pimephales promelas (Veith et al. 1983)

793 • Dichlorvos 62-73-7

D

Synonyms	2,2-Dichlorovinyl-0,0-dimethyl phosphate DDVP	
Use	Active ingredient in insecticides.	
State and appearance	Colourless to amber liquid.	
Molecular weight	220.98	
Vapour pressure, mmHg	0.012	20 °C
Boiling point, °C	35–120	
LD50 values to mammals in oral exposure, mg/kg	32 10	orl-rat orl-rbt (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	70.4 107	skn-rat skn-rbt (Lewis & Sweet 1984)
Carcinogenicity	NCI carcinogenesis bioassay completed: results negative; mus, rat (Lewis & Sweet 1984).	
LD50 values to birds in oral exposure, mg/kg	13.3–17.8 11.0–42.2 23.7 17.8 13.3 23.7	orl-Agelaius phoeniceus orl-Sturnus vulgaris orl-Coturnix coturnix orl-Passer domesticus orl-Quiscalus quiscala orl-Columba livia (Schafer et al. 1983)
LC50 values to crustaceans, mg/l	0.00026	48hr, Simocephalus serrulatus (Sanders & Cope 1966)
	0.881	96hr, Macrobrachium lamarrei (Omkar & Shukla 1985)
	0.0004	96hr, Gammarus fasciatus (Sanders 1972)
	0.009	act, Daphnia pulex (Nishiuchi & Hashimoto 1967)
	0.02 0.01	24hr, Daphnia magna act, 48hr (Ardo 1974)
	0.000066	act, Daphnia pulex (Kenaga 1979)
	0.0131 0.0083 0.0058	1d, Macrobrachium lamarrei 2d, Macrobrachium lamarrei 3d, Macrobrachium lamarrei (Mary et al. 1986)

LC50 values to fishes, mg/l	0.2	96hr, Mugil cephalus (Eisler 1970a)
	0.87	96hr, Lepomis macrochirus (Verschueren 1983)
	0.4	96hr, Mystus vittatus (Verma et al. 1981a)
	2.04	96hr, Channa punctata (Verma et al. 1981a)
	1	24hr, Lepomis macrochirus (Pesticide Manual 1983)
	0.48	act, Lepomis macrochirus (Kenaga 1979)
	> 40	48hr, Cyprinus carpio (Nishiuchi & Hashimoto 1967)
Effects on the physiology of water organisms	Lamellidens marginalis; 5 mg/l, 2d, biochemical effect (change in physiochemical process including glycogen uptake, cholesterol levels and lipid analysis) (Srinavasamoorthy et al. 1986). Tilapia mossambica; 0.014 mg/l, 90d, change in growth (Pal & Konar 1986).	
Other information about water organisms	LC50 0.0001 mg/l, 96hr, Pteronarcys californica (Sanders & Cope 1968).	

794 • Dichlorvos-ethyl

72-00-4

Other information about mammals	ALD = 42.0 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987).

795 • Dicrotophos (cis(E)-isomer)

141-66-2

Other information about mammals	LDfr = 25.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).	
LD50 values to birds in oral exposure, mg/kg	00–1.60	orl-Agelaius phoeniceus
	2.70–10.0	orl-Sturnus vulgaris
	7.5	orl-Coturnix coturnix
	4.22	orl-Passer domesticus
	1.78	orl-Quiscalus quiscula
	4.22	orl-Columba livia
	1.33	orl-Quelea quelea (Schafer et al. 1983)

796 • Dicrotophos (Z-isomer)

18250-63-0

Use	Insecticide, acaricide.	
LC50 values to crustaceans, mg/l	0.6	Daphnia pulex (Kenaga 1979)
LC50 values to fishes, mg/l	6.3	act, Salmo gairdneri (Kenaga 1979)

797 • 1,3-Dicyanobenzene

626-17-5

Sumformula of the chemical	C8H4N2
Melting point, °C	161.5 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).

Bioconcentration factor, fishes	< 0.57–2.1 6w, Cyprinus carpio, conc 0.5 mg/l > 5.6 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
LC50 values to fishes, mg/l	180 48hr, Oryzias latipes (MITI 1992)

798 • 1,4-Dicyanobenzene 623-26-7

Synonyms	Terephtalonitrile
Water solubility, mg/l	< 10 (MITI 1992)
Melting point, °C	222 (MITI 1992)
Log octanol/water coefficient, log Pow	1.2 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	0.68–1.3 6w, Cyprinus carpio, conc 0.1 mg/l < 1.5–2.0 6w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	> 50 48hr, Oryzias latipes (MITI 1992)

799 • 1,6-Dicyanohexane 629-40-3

LC50 values to fishes, mg/l	528 96hr, Pimephales promelas (Broderius & Kahl 1985)

800 • Dicyclohexyl amine 101-83-7

Melting point, °C	0.1 (MITI 1992)
Boiling point, °C	255.8 (MITI 1992)
Total degradation in water	Biodegradation: 76.9% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

801 • Dicyclohexyl phthalate 84-61-7

Synonyms	Benzene-1,2-dicarboxylic acid dicyclohexyl
Melting point, °C	64 (MITI 1992)

Total degradation in water	Biodegradation: 68.5% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

802 • N,N'-Dicyclohexyl thiourea 1212-29-9

Water solubility, mg/l	< 10	(MITI 1992)
Melting point, °C	180–182 (MITI 1992)	
Log octanol/water coefficient, log Pow	3.69	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	1.4–5.7 < 4.4	6w, Cyprinus crpio, conc 0.1 mg/l 6w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	> 500	48hr, Oryzias latipes (MITI 1992)

803 • Dicyclohexylcarbodiimide 538-75-0

Water solubility, mg/l	10	(MITI 1992)
Boiling point, °C	129–131 3 mmHg (MITI 1992)	
Total degradation in water	Biodegradation: 0–1% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	0.2–0.7 < 2.2	6w, Cyprinus carpio, conc 1 mg/l 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	> 250	48hr, Oryzias latipes (MITI 1992)

804 • 2,6-Dicyclohexylphenol 4821-19-6

Sumformula of the chemical	C18H26O	
Water solubility, mg/l	7	(MITI 1992)
Melting point, °C	75.5	(MITI 1992)

Log octanol/water coefficient, log Pow	> 6.19 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	919–3140 8w, Cyprinus carpio, conc 0.015 mg/l 384–1170 8w, Cyprinus carpio, conc 0.0015 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be accumulated on a medium level (Anon. 1987).
LC50 values to fishes, mg/l	6.5 48hr, Oryzias latipes (MITI 1992)

D

805 • N,N'-Dicyclohexylurea 2387-23-7

Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).

806 • Dicyclopentadiene 77-73-6

Synonyms	Bicyclopentadiene
Odour	Quality: sweet, sharp Hedonic tone: unpleasant Threshold odour concentration absolute: 0.011 ppm 50% recognition: 0.020 ppm 100% recognition: 0.020 ppm Odour index 100% recognition: 440 500 (Hellman & Small 1974).
Melting point, °C	33.6 (MITI 1992)
Boiling point, °C	170 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	112–330 8w, Cyprinus carpio, conc 0.3 mg/l 58.9–384 8w, Cyprinus carpio, conc 0.03 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non–accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	3.7 48hr, Oryzias latipes (MITI 1992)

807 • DID 100 7393-66-0

Other information about mammals	LDfr = 100 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

808 • Didecyl disulfide

10496-18-1

Sumformula of the chemical	C20H42S2	
Water solubility, mg/l	< 56000	(MITI 1992)
Melting point, °C	14.3	(MITI 1992)
Log octanol/water coefficient, log Pow	> 5.75	(MITI 1992)
Total degradation in water	Biodegradation: 2–5% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 4.5 < 45	6w, Cyprinus carpio, conc 0.5 mg/l 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 500	48hr, Oryzias latipes (MITI 1992)

809 • Dieldrin

60-57-1

Synonyms	1,2,3,4,10,10-Hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a-octahydro-exo-1,4-endo-5,8-dimethanonaphthalene HEOD	
Sumformula of the chemical	C12H8Cl6O	
Products containing the chemical	Compound 497 HEOD Octalox	
Use	Insecticide in agriculture and forestry; handling of textiles; spraying of unpeeled timber.	
Molecular weight	380.9	
Density, kg/m³	1750	
Vapour pressure, mmHg	0.00000018, 25 °C	
Water solubility, mg/l	0.19 0.14	25 °C (MITI 1992)
Melting point, °C	176–177 (MITI 1992)	
Log octanol/water coefficient, log Pow	5.48 3.69 5.48 5.61	(Anon. 1988) (Anon. 1989) (Mackay 1982) (MITI 1992)
Henry's law constant, Pa x m³/mol	0.091 1.12	(Anon. 1988) 20 °C (Anon. 1989)
Photochemical degradation in water	Photooxidation by UV-radiation in aqueous medium (90–95 °C): 75% CO2 in 12.5 hours (Knoevenagel & Himmelreich 1976).	
Half-life in soil, days	868	(Li et al. 1990)
Half-life in water, days	539	calculated, 25 °C (Verschueren 1983)
Total degradation in soil	Time for 95% disappearance from the soil (3.1–5.6 kg/ha): 12.8 years (Caro et al. 1975/1976). 70–100% disappearance from soils: 3–25 years. (Verschueren 1983)	

D

Total degradation in water	Persistance in river water in a sealed glass jar in sunlight: 100% left after 8 weeks (Eichelberger & Lichtenberg 1971). Biodegradation: 0% by BOD period: 17.5d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Other information about degradation	Not easily biodegradable (Anon. 1989). Degradation products of special interest: stereoisomer to endrin; photodieldrin (Anon. 1989).
Metabolism in mammals	Uptake via respiratory tract, skin and alimentary canal, deposited in fat tissue (USEPA 1980).
Bioconcentration factor, fishes	3300 Salmo trutta (Verschueren 1983) 4430 Pseudorasbora (Kanazava 1983) 4860–14500 10w, Cyprinus carpio, conc 0.001 mg/l 5390–12500 10w, Cyprinus carpio, conc 0.0001 mg/l (lipid content 7.0%) 3940–10200 10w, Cyprinus carpio, conc 0.001 mg/l 4170–12800 10w, Cyprinus carpio, conc 0.0001 mg/l (lipid content 1.7%) (MITI 1992)
Bioconcentration factor, mollusca	700–5500 (Verschueren 1983) 5100–5500 43d, Crassostrea (Emanuelsen et al. 1978)
Bioconcentration factor, algae	16000 2hr, Skeletonema 4800 2hr, Cyclotella (Rice & Sikka 1973)
Other information about bioaccumulation	Confirmed to be accumulated on a high level (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	38.3 orl-rat 65 orl-dog 3 orl-mky (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	10 skn-rat (Lewis & Sweet 1984) 46 ukn-rat (Virtanen & Nuuja 1987)
Other information about mammals	LC50 66–132 mg/kg, 14 days, Blarina brevicauda (Virtanen & Nuuja 1987) Lethal dose in brains: (Virtanen & Nuuja 1987) bat: 5.0–10.0 mg/kg rat: 2.1–10.8 mg/kg dog: 2.4–9.4 mg/kg rabbit: 8.4–19.1 mg/kg
Health effects	Lethal dose to human 70 mg/kg (Virtanen & Nuuja 1987). Effects on central nervous system, liver, kidneys and skin (USEPA 1980).
Carcinogenicity	Carcinogen (McCann et al. 1975). NCI carcinogenesis bioassay completed: result indefinite, mus; result negative, rat (Lewis & Sweet 1984).
Mutagenicity	No Ames-mutagen (McCann et al. 1975).
Teratogenicity	Decreased fertility, embryo mortality and/or mortality of newborn, 0.015–0.125 mg/kg in day (oral) (USEPA 1987).

LD50 values to birds in oral exposure, mg/kg	20	orl-ckn
	23	orl-bwd
	27	orl-pgn (Lewis & Sweet 1984)
	17.8	orl-Agelaius phoeniceus
	237	orl-Sturnus vulgaris
	56.2	orl-Coturnix coturnix
	13.3	orl-Passer domesticus
	42.2	orl-Quiscalus quiscula
	23.7	orl-Columba livia (Schafer et al. 1983)
LC50 values to crustaceans, mg/l	0.23	48hr, Daphnia magna (Gorbach & Knauf 1971)
	0.46	96hr, Gammarus lacustris (Sanders 1969)
	0.005	96hr, Asellus brevicaudus
	0.02	96hr, Palaemonetes kadiakensis (Sanders 1972)
	0.25	48hr, Daphnia pulex (Sanders & Cope 1966)
	2.5	act, Daphnia pulex (Frear et al. 1967)
	> 0.2	24hr, Daphnia magna
	> 0.2	48hr, Daphnia magna (Adema 1978)
	0.33	act, Daphnia magna (Kenaga 1979)
		technical material, 85% HEOD:
	0.005	96hr, 21 °C, Asellus, mature
	0.64	96hr, 21 °C, Gammarus fasciatus, mature (Johnson & Finley 1980)
EC50 values to crustaceans, mg/l	0.251	srv, act, Daphnia pulex (Daniels & Allan 1981)
	0.25–0.33	Daphnia pulex (Shapiro 1979)
		technical material, 85% HEOD:
	0.24	48hr, 15 °C, Simocephalus, first instar
	0.19	48hr, 15 °C, Daphnia pulex, first instar (Johnson & Finley 1980)
NOEC values to crustaceans, mg/l	0.1	srv, Daphnia magna
	0.32	rpd, Daphnia magna (Adema 1978)

LC50 values to fishes, mg/l	0.0009	96hr, Anguilla rostrata (Eisler 1970a)
	0.0002	96hr, Acroneurica pacifica (Jensen & Gaufin 1966)
	0.016	96hr, Pimephales promelas
	0.008	96hr, Lepomis macrochirus (Henderson et al. 1959)
	0.003	135d, Poecilia latipinna (Lane & Livingston 1970)
	0.019	96hr, Salmo gairdneri
	0.008	96hr, Lepomis macrochirus (Edwards 1977)
	0.003	act, Lepomis macrochirus
	0.001	act, Salmo gairdneri
	0.004	act, Pimephales promelas (Kenaga 1979)
	0.01	96hr, Salmo gairdneri
	0.006	96hr, Oncorhynchus tschawytscha (Katz 1961)
	0.0045	96hr, Ictalurus (Anon. 1989)
		technical material, 85% HEOD:
	0.006	96hr, 9 °C, hrd, Salmo clarci
	0.0012	96hr, 13 °C, Salmo gairdneri
	0.0018	96hr, 18 °C, Carassium auratus
	0.0038	96hr, 18 °C, Pimephales promelas
	0.0045	96hr, 18 °C, Ictalurus punctatus
	0.0031	96hr, 18 °C, Lepomis macrochirus
	0.0035	96hr, 18 °C,hrd, Micropterus salmoides
		photo-dieldrin 98%:
	0.012	96hr, 8 °C,hrd, Salmo clarci
	0.019	96hr, 18 °C, Ictalurus punctatus
	0.011	96hr, 18 °C, Lepomis macrochirus (Johnson & Finley 1980)
	27.5	48hr, Oryzias latipes (MITI 1992)
LOEC values to fishes, mg/l	0.00075	grw, rpd, schr, 240d, Poecilia latipinna (Lane & Livingston 1970)
Effects on the physiology of water organisms	Sphaerium corneum, 6d, 0.002 mg/l, enzyme effect (Boryslawskyj et al. 1988).	
	Dietary dieldrin significantly altered several physiological and biochemical factors, including serum amino acid composition, adrenal and thyroid function, ammonia detoxification, and phenylketo acid metabolism. The ability to withstand stress was significantly reduced. Whole body residues in treated fish were similar to those in wild fish (Johnson & Finley 1980).	
Other information about water organisms	Chironomus riparius, 24hr, LC50, 0.0005 mg/l (Estenik & Collins 1979).	
	Lepomis gibbosus, 100d, influence on swimming and oxygen intake, 0.0017 mg/l (Cairns & Scheier 1964).	
	Poecilia latipinna, 34 weeks, decreaced growth and reproduction (Lane & Livingston 1970).	
	LC50, 96hr, technical material, 85% HEOD: Orconectes, 21 °C, 0.740 mg/l, mature; Pteronarcys, 15 °C, 0.0005 mg/l, second year class; Pteronarcella, 15 °C, 0.0005 mg/l, first year class; Claassenia, 15 °C, 0.0006 mg/l, second year class; Ischnura, 24 °C, 0.012 mg/l, juvenile (Johnson & Finley 1980).	
Other information	Stereo-isomer of endrin, oxidation product of aldrin (EPA 1975).	
	Production forbidden in USA in 1974 (Anon. 1989).	

810 • Diethanolamine 111-42-2

Synonyms	Diethylolamine DEA Bis(2-hydroxyethyl)amine	
Use	Liquid detergents for emulsion points, cutting oils, shampoos; chemical intermediate for resin; plasticizers; solvent.	
Molecular weight	105.16	
Vapour pressure, mmHg	< 0.01	20 °C
Water solubility, mg/l	950000 soluble	20 °C (MITI 1992)
Melting point, °C	28	(MITI 1992)
Boiling point, °C	269.1	(MITI 1992)
Volatilization	5% converted to CO2 in days in stream water (initial conc. 21 mg/l) (Verschueren 1983). Relative volatility (nBuAc=1) = < 0.001	
Chemical oxygen demand, g O2/g	1.52	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g O2/g	0.03	5 days (Bridie et al. 1979)
Total degradation in water	Biodegratation: 51.4% by BOD (on the upward trend) period: 21d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	710 2	orl-rat orl-gpg (Lewis & Sweet 1984)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): > 10000 mg/l (Bringmann & Kühn 1980a)	
LOEC values to algae, mg/l	4.4	Scenedesmus quadricauda (Bringmann & Kuhn 1980a)
LC50 values to crustaceans, mg/l	1.4 55	act, Daphnia magna (Verschueren 1983) 48hr, Daphnia magna (LeBlanc 1980)
LC50 values to fishes, mg/l	> 5000	24hr, Carassius auratus (Bridie et al. 1979)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 4.4 mg/l protozoa (Entosiphon sulcatum): 160 mg/l (Bringmann & Kühn 1980a)	

811 • O,O-Diethyl O-(3,5,6-trichloro-2-pyridyl) phosphorothioate

2921-88-2

Synonyms	Chlorpyrifos Brodan Dowco 179 Dursban Eradex Lorsban
Sumformula of the chemical	C9H11Cl3NO3PS
Use	Active ingredient in insecticides.
State and appearance	Amber solid cake with amber oil.
Molecular weight	350.59
Specific gravity (water=1)	1.398 at 43.5 °C
Vapour pressure, mmHg	0.0000187 20 °C
Water solubility, mg/l	0.4 23 °C 1 (MITI 1992)
Melting point, °C	42.0–43.5 (MITI 1992)
Degradation point, °C	160
Log octanol/water coefficient, log Pow	5.11 at 20 °C 4.6 (Anon. 1988)
Log soil sorption coefficient, log Kom	4.13 (Sabljic 1987)
Henry's law constant, Pa x m³/mol	0.44 (Anon. 1988)
Mobility	Equilibrium distribution *mass %* air 2.08 water 13.78 solid 84.14 (Anon. 1988)
Hydrolysis in water	Half-life 35.5 days at pH 6.9, 25 °C (Verschueren 1983). A 16-fold rate enhancement was demonstrated in canal and pond water at 25 °C qualitatively the products of hydrolysis were: 3,5,6-trichloro-2-pyridinol O-ethyl, O-hydrogen-O-(3,5,6-trichloro-2-pyridyl)phosphorothioate O, O-dihydrogen-O-(3,5,6-trichloro-2-pyridyl)phosphorothioate (Meikle & Youngson 1978)
Hydrolysis in acid	Half-life 62.7 days at pH 4.7, 25 °C (Verschueren 1983)
Hydrolysis in base	Half-life 22.8 days at pH 8.1, 25 °C (Verschueren 1983)
Half-life in soil, days	63 (Li et al. 1990)
Total degradation in soil	Persistance in soil (10 ppm initial conc.):

	weeks incubation to	
	50% remaining	*5% remaining*
sterile sandy loam	17	-
sterile organic soil	> 24	-
non sterile sandy loam	< 1	1
non sterile organic soil	2.5	8

(Miles et al. 1979)

Total degradation in water	Biodegradation: 0.2% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992)
Bioconcentration factor, fishes	468 Salmo gairdneri (Verschueren 1983) 853–2880 (8w, Cyprinus carpio, conc 0.01 mg/l 49–493 8w, Cyprinus carpio, conc 0.001 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be accumulated on a medium level (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	97 orl-rat 60 orl-mus 152 orl-mus 1000 orl-rbt (Lewis & Sweet 1984) 163 orl-male-rat (Verschueren 1983) 135 orl-female-rat (Verschueren 1983) 500 orl-gpg (Verschueren 1983) 1000–2000 orl-rbt (Nimmo et al. 1979)
LD50 values to mammals in non-oral exposure, mg/kg	202 skn-rat 2000 skn-rbt 78 ihl-rat (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	8 orl-bwd 16 orl-qal 25 orl-ckn 76 orl-dck (Lewis & Sweet 1984) 13.3 orl-Agelaius phoeniceus 75 orl-Sturnus vulgaris 13.3 orl-Coturnix coturnix 10 orl-Passer domesticus 5.62–13.3 orl-Quiscalus quiscula 10 orl-Columba livia 8.4 orl-Phasianus colchicus 31.6 orl-Corvus brachyrhynchos (Schafer et al. 1983)
Effects on arthropods	LC50 0.01 mg/l, 96hr, Pteronarcys californica LC50 0.00038 mg/l, 96hr, Pteronarcella badia LC50 0.00057 mg/l, 96hr, Classenia sabulosa (Sanders & Cope 1968)
EC50 values to algae, mg/l	0.228–0.402 96hr, Skeletonema costatum (Borthwick & Walsh 1981)
LC50 values to crustaceans, mg/l	0.0017 Daphnia magna (Kenaga 1979) 0.00001 96hr, Palaemon macrodactylus (Verschueren 1983 0.00011 96hr, Gammarus lacustris (Sanders 1969) 0.00006 96hr, Mysidopsis bahia (Borthwick & Walsh 1981) 0.006 96hr, Orconectes nais (Phipps & Holcombe 1985) 0.00032 96hr, Gammarus fasciatus (Sanders 1972)

D

LC50 values to fishes, mg/l	0.003	Salmo gairdneri (Pesticide Manual 1983)
	0.0026	96hr, Lepomis macrochirus
	0.011	96hr, Salmo gairdneri (Verschueren 1983)
	0.0047	96hr, Fundulus heteroclitus (Thirugnanam & Forgash 1977)
	0.203	96hr, Pimephales promelas
	0.008	96hr, Salmo gairdneri (Holcombe et al. 1982)
	0.009	96hr, Salmo gairdneri
	0.01	96hr, Lepomis macrochirus
	0.542	96hr, Pimephales promelas
	> 0.806	96hr, Carassius auratus
	0.806	96hr, Ictalurus punctatus (Phipps & Holcombe 1985)
	0.0033	act, Lepomis macrochirus
	0.003	act, Salmo gairdneri (Kenaga 1979)
	0.04	72hr, Lepomis cyanellus
	0.26	72hr, mosquitofish (Davey et al. 1976)
	1	48hr, Oryzias latipes (MITI 1992)
LOEC values to fishes, mg/l	0.00012	grw, chr, Pimephales promelas
	0.0027	phy, chr, Pimephales promelas
	0.005	srv, grw, schr, Pimephales promelas (Järvinen et al. 1983)
Other information about water organisms	LC50 (96hr), 0.000038 mg/l, Pteronarcella badia (Sanders & Cope 1968) LC50, > 0.806 mg/l, 96hr, snail (Phipps & Holcombe 1985)	

812 • Diethyl biphenyl 28575-17-9

Sumformula of the chemical	C16H18	
Water solubility, mg/l	> 10	(MITI 1992)
Boiling point, °C	300–330	(MITI 1992)
Total degradation in water	Biodegradation: 61–77% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).	
Bioconcentration factor, fishes	2600–11800	8w, Cyprinus carpio, conc 0.05 mg/l
	930–4440	8w, Cyprinus carpio, conc 0.05 mg/l
	676–3790	8w, Cyprinus carpio, conc 0.05 mg/l
	753–4150	8w, Cyprinus carpio, conc 0.05 mg/l
	3790–14600	8w, Cyprinus carpio, conc 0.005 mg/l
	1040–5320	8w, Cyprinus carpio, conc 0.005 mg/l
	885–3930	8w, Cyprinus carpio, conc 0.005 mg/l
	878–4420	8w, Cyprinus carpio, conc 0.005 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be accumulated on a medium level (Anon. 1987).	
LC50 values to fishes, mg/l	8.2	48hr, Oryzias latipes (MITI 1992)

813 • Diethyl carbonate 105-58-8

Synonyms	Ethyl carbonate
Sumformula of the chemical	C5H10O3
Use	Solvent for nitrocellulose, cellulose ethers, many synthetic and natural resins; organic synthesis; adhering rare earths to cathodes.
State and appearance	Colourless liquid.
Odour	Mild odour.
Boiling point, °C	125
Log octanol/water coefficient, log Pow	1.21 (Sangster 1989)
Other physicochemical properties	Miscible with alcohols, ketones, esters, aromatic hydrocarbons, some aliphatic solvents; insoluble in water. Combustible. Flammable, dangerous fire risk.

814 • O,O-Diethyl dithiophosphate 298-06-6

Sumformula of the chemical	C4H11O2PS2	
Water solubility, mg/l	64000	(MITI 1992)
Melting point, °C	≤ 10	(MITI 1992)
Log octanol/water coefficient, log Pow	-0.77	(MITI 1992)
Total degradation in water	Biodegradation: 0–3% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.5 < 5.0	6w, Cyprinus carpio, conc 1 mg/l 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
LC50 values to fishes, mg/l	440	48hr, Oryzias latipes (MITI 1992)

815 • Diethyl sulfate 64-67-5

Melting point, °C	-24.5	(MITI 1992)
Boiling point, °C	208	760 mmHg (MITI 1992)
Total degradation in water	Biodegradation: 49% (on the upward trend) by BOD 89% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	

816 • O,O-Diethyl-O-(4-nitrophenyl) phosphorothioate

56-38-2

Synonyms	O,O-Diethyl-O-(p-nitrophenyl) phosphorothioate Diethyl p-nitrophenyl thiophosphate Diethylparathion Ecatox Ekatox Ethyl parathion Parathion-ethyl Sulphos Thiophos Parathion	
Use	Active ingredient in insecticides, acaricide, avicide.	
Molecular weight	291.28	
Vapour pressure, mmHg	0.003	24 °C
Water solubility, mg/l	24	
Melting point, °C	375	
Boiling point, °C	157–162	
Log octanol/water coefficient, log Pow	3.8 3.81	(Anon. 1988) (Schwarzenbach & Westall 1981)
Log organic C/water coefficient, log Pcw	3.06 3.23	exptl (Schwarzenbach & Westall 1981) calcd (Schwarzenbach & Westall 1981)
Log soil sorption coefficient, log Kom	3.68	(Sabljic 1987)
Henry's law constant, Pa x m³/mol	0.0076	(Anon. 1988)
Mobility	Equilibrium distribution: air water solid	 *mass %* 0.13 50.75 49.13 (Anon. 1988)
Half-life in soil, days	18	(Li et al. 1990)
Total degradation in soil	75–100% disappearance from soils: 1 week (Verschueren 1983) 5% remaining after 10 weeks incubation (nonsterile organic soil) (Verschueren 1983)	
Total degradation in water	< 5% of original compound found after 4 weeks in river water (initial concentration 0.010 mg/l) (Verschueren 1983)	
Bioconcentration factor, fishes	80	(Verschueren 1983)
Bioconcentration factor, mollusca	50	(Verschueren 1983)
LD50 values to mammals in oral exposure, mg/kg	2 0.93 6	orl-rat orl-cat orl-mus (Lewis & Sweet 1984)

LD50 values to mammals in non-oral exposure, mg/kg	6.8 skn-rat 1.5 ipr-rat 6 ims-rat 32.4 skn-mus 5.6 ipr-mus 3.55 ipr-rat 11.5 scu-mus 17.4 ivn-mus 7.2 ims-mus (Lewis & Sweet 1984)
LDLo values to mammals in oral exposure, mg/kg	0.24 orl-hmn (Lewis & Sweet 1984)
LDLo values to mammals in non-oral exposure, mg/kg	3 ivn-rat (Lewis & Sweet 1984)
LCLo values to mammals in inhalation exposure, mg/kg	10 ihl-rat, 2hr (Lewis & Sweet 1984)
TDLo values to mammals in oral exposure, mg/kg	5.67 orl-wmn (Lewis & Sweet 1984)
Carcinogenicity	NCI carcinogenesis bioassay completed: results indefinite, rat; results negative, mus (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	2 orl-bwd 2.1 orl-dck (Lewis & Sweet 1984) 2.37 orl-Agelaius phoeniceus 5.62 orl-Sturnus vulgaris 4.22 orl-Coturnix coturnix 1.33 orl-Passer domesticus 5.62 orl-Quiscalus quiscula 1.33 orl-Columba livia 2.37 orl-Carpodacus mexicanus 1.33 orl-Molothrus ater 1.78 orl-Quelea quelea 1.78 orl-Ploceus cucullatus (Schafer et al. 1983)
LD50 values to birds in dermal exposure, mg/kg	1.8 skn-bwd (Lewis & Sweet 1984)
Effects on arthropods	LC50 (96hr), 0.00016 mg/l, Ephemerella subvaria LC50 (30d), 0.000013 mg/l, Acroneurica lycorias (Verschueren 1983).
LC50 values to crustaceans, mg/l	0.0006 48hr, Daphnia pulex 0.0004 48hr, Daphnia magna (Sanders & Cope 1966) 0.0021 96hr, Gammarus fasciatus 0.0016 120hr, Gammarus fasciatus 0.00004 96hr, Orconectes nais (Sanders 1972) 0.008 act, Daphnia pulex (Hashimoto & Nishiuchi 1981) 0.0035 21d, Daphnia magna (Dortland 1978) 0.0008 48hr, Daphnia magna (Frear & Boyd 1967) 0.00076 48hr, Daphnia pulex (Priester 1966) 0.0008 act, Daphnia pulex (Nishiuchi & Hashimoto 1967) 0.008 act, Daphnia magna (Kenaga 1979) 0.003–0.01 48hr, Crangon crangon (Kemp et al. 1973)

D

LC50 values to fishes, mg/l	1.4–2.7 1.5	96hr, Pimephales promelas 96hr, Salmo gairdneri (Pesticide Manual 1983)
	0.047 2 1.9	act, Lepomis macrochirus act, Salmo gairdneri act, Pimephales promelas (Kenaga 1979)
	1.4	96hr, Pimephales promelas (Solon & Nair 1970)
	0.065	96hr, Lepomis macrochirus (Pickering et al. 1962)
	4.5 1.7	48hr, Cyprinus carpio 48hr, Carassius auratus (Hashimoto & Nishiuchi 1981)
	1.8	96hr, Pimephales promelas (Priester 1966)
	3.2	48hr, Cyprinus carpio (Nishiuchi & Hashimoto 1967)
Other information about water organisms	Chironomus riparius, LC50, 0.211 mg/l, 1 d (Fisher & Lohner 1987)	

D

817 • N, N-Diethyl-3-toluamide 134-62-3

Synonyms	Diethyltoluamide N, N-Diethyl-m-toluamide	
Water solubility, mg/l	> 1000	(MITI 1992)
Boiling point, °C	160	(MITI 1992)
Log octanol/water coefficient, log Pow	2.66	(MITI 1992)
Total degradation in water	Biodegradtion: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	0.8–2.4 < 2.4	6w, Cyprinus carpio, conc 0.5 mg/l 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LD50 values to birds in oral exposure, mg/kg	> 500	orl-Agelaius phoeniceus (Schafer et al. 1983)
LC50 values to fishes, mg/l	100	48hr, Oryzias latipes (MITI 1992)

818 • Diethylamine 109-89-7

Sumformula of the chemical	C4H11N
Use	Solvent.

Odour	Quality: musty, fishy, amine Hedonic tone: unpleasant Threshold odour concentration absolute: 0.02 ppm 50% recognition: 0.06 ppm 100% recognition: 0.06 ppm Odour index 100% recognition: 4 250 000 (Hellman & Small 1974).	
Water solubility, mg/l	815000 > 100	20 °C (MITI 1992)
Melting point, °C	-50	(MITI 1992)
Boiling point, °C	55	(MITI 1992)
pKa	11.07	(Sangster 1989)
Log octanol/water coefficient, log Pow	0.58	(Sangster 1989)
Henry's law constant, Pa x m³/mol	6.672	calc. (Yaws et al. 1991)
Volatilization	Relative volatility (nBuAc=1) = 16.9	
Total degradation in water	Biodegradation: 68–70% by BOD substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
LD50 values to mammals in oral exposure, mg/kg	540	orl-rat
LC50 values to algae, mg/l	20	96hr, Selenastrum capricornutum (Calamari et al. 1982b)
LC50 values to crustaceans, mg/l	164	24hr, Daphnia magna (Calamari et al. 1982b)
LC50 values to fishes, mg/l	25	96hr, Salmo gairdneri (Calamari et al. 1980)

819 • Diethylaminoethylchloride-HCl 869-24-9

Other information about mammals	LDfr = 100 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).	
LD50 values to birds in oral exposure, mg/kg	42.2 100	orl-Agelaius phoeniceus orl-Sturnus vulgaris (Schafer et al. 1983)

820 • 4-Diethylaminosalicylaldehyde 17754-90-4

LC50 values to fishes, mg/l	5.36	96hr, Pimephales promelas (Broderius & Kahl 1985)

821 • N, N-Diethylaniline 91-66-7

Sumformula of the chemical	C10H15N	
Boiling point, °C	216.5	(MITI 1992)
pKa	6.55	(Sangster 1989)

Log octanol/water coefficient, log Pow	3.31 (Sangster 1989)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Bioconcentration factor, fishes	44–161 8w, Cyprinus carpio, conc 0.2 mg/l 17–125 8w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	16.8 48hr, Oryzias latipes (MITI 1992)

822 • 1,2-Diethylbenzene 135-01-3

Synonyms	o-Diethylbenzene
Other information about water organisms	LOEC 6.9 mg/l, rpd, schr, Entosiphon sulcatum (Bringmann & Kühn 1980a).

823 • 1,3-Diethylbenzene 141-93-5

Synonyms	m–Diethylbenzene
Sumformula of the chemical	C10H14
EINECS-number	2055114
Water solubility, mg/l	24 (MITI 1992)
Melting point, °C	< -10 (MITI 1992)
Boiling point, °C	181–182 (MITI 1992)
Log octanol/water coefficient, log Pow	4.43 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	350–854 6w, Cyprinus carpio, conc 0.02 mg/l 413–653 6w, Cyprinus carpio, conc 0.002 mg/l (MITI 1992)
LC50 values to fishes, mg/l	3.97 48hr, Oryzias latipes (MITI 1992)

824 • 1,4-Diethylbenzene 105-05-5

Synonyms	p–Diethylbenzene
Sumformula of the chemical	C10H14

EINECS-number	2032652
Water solubility, mg/l	17 (MITI 1992)
Melting point, °C	< -10 (MITI 1992)
Boiling point, °C	182–183 (MITI 1992)
Log octanol/water coefficient, log Pow	4.6 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	362–598 6w, Cyprinus carpio, conc 0.02 mg/l 320–629 6w, Cyprinus carpio, conc 0.002 mg/l (MITI 1992)
LC50 values to fishes, mg/l	2.49 48hr, Oryzias latipes (MITI 1992)

825 • Diethylene glycol

111-46-6

Synonyms	DEG Diglycol Bis(2-hydroxyethyl)ether Dihydroxydiethyl ether β,β'-Dihydroxydiethyl ether 2,2'-Dihydroxydiethyl ether 2,2'-Oxydiethanol Ethylene diglycol Glycol ether Glycolethyl ether 3-Oxapentane-1,5-diol 3-Oxa-1,5-pentanediol 2,2'-Oxybisethanol
Sumformula of the chemical	C4H1003
Molecular weight	106.14
Water solubility, mg/l	> 100000 (MITI 1992)
Melting point, °C	-6.5 (MITI 1992)
Boiling point, °C	245 (MITI 1992)
Chemical oxygen demand, g 02/g	1.51 5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.05 5 days (Bridie et al. 1979)
Total degradation in water	Biodegradation: 82–98% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).

LD50 values to mammals in oral exposure, mg/kg	3300 9000 7800 1000 23700 12565 4400	orl-cat orl-dog orl-gpg orl-hmn orl-mus orl-rat orl-rbt (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	9719 6565 11890	ipr-mus ivn-rat skn-rbt (Sweet 1987)
LDLo values to mammals in non-oral exposure, mg/kg	7826 4472 2236 5000 16770	ims-rat ims-rbr ivn-rbt scu-mus scu-rat (Sweet 1987)
LCLo values to mammals in inhalation exposure, mg/kg	130	ihl-mus, 2hr (Sweet 1987)
TDLo values to mammals in oral exposure, mg/kg	890000 50000	orl-rat, tumorigenic orl-rat, 1-20d preg. specific developmental abnormalities (Sweet 1987)
Other information about mammals	Skin and eye irritation data: skin, human, 112 mg, mild; skin, rabbit, 500 mg, mild; eye, rabbit, 50 mg, mild (Sweet 1987).	
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 8000 mg/l (Bringmann & Kühn 1980a)	
EC50 values to microorganism, mg/l	29000	15 min Microtox (Hermens et al. 1985)
LOEC values to algae, mg/l	1700	rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to crustaceans, mg/l	0.3–1.0	act, Daphnia magna (Verschueren 1983)
LC50 values to fishes, mg/l	> 5000	24hr, Carassius auratus (Bridie et al. 1979)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 2700 mg/l protozoa (Entosiphon sulcatum): 10745 mg/l (Bringmann & Kühn 1980a).	

826 • Diethylene glycol mono-n-butyl ether 112-34-5

Synonyms	Diethylene glycol monobutylether 1-n-Butoxy-3-oxabutan-5-ol	
Sumformula of the chemical	C8H18O3	
EINECS-number	2039616	
Water solubility, mg/l	> 100000 (MITI 1992)	
Melting point, °C	-68.1	(MITI 1992)
Boiling point, °C	230.4	(MITI 1992)

Chemical oxygen demand, g 02/g	2.08	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.25	5 days (Bridie et al. 1979)
Total degradation in water	Biodegradation: 89–93% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
LOEC values to algae, mg/l	53	rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1980a)
LC50 values to fishes, mg/l	2700	24hr, Carassius auratus (Bridie et al.1979)
	1300	96hr, Lepomis macrochirus (Dawson et al. 1977)
Other information about water organisms	LOEC 73 mg/l, rpd, schr, Entosiphon sulcatum (Bringmann & Kühn 1980a).	

D

827 • Diethylene glycol monoethyl ether acetate 112-15-2

Sumformula of the chemical	C8H16O4	
EINECS-number	2039401	
Water solubility, mg/l	> 100000 (MITI 1992)	
Melting point, °C	-25	(MITI 1992)
Boiling point, °C	218	(MITI 1992)
Total degradation in water	Biodegradation: 98–103% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

828 • Diethyleneglycol diethylether 112-36-7

LC50 values to crustaceans, mg/l	6600	96hr, Nitocra spinipes (Linden et al.1979)
LC50 values to fishes, mg/l	> 10000	96hr, 10 °C, Alburnus alburnus (Linden et al. 1979)

829 • Diethyleneglycol monoethylether 111-90-0

Synonyms	1-Ethoxy-3-oxabutan-5-ol	
Chemical oxygen demand, g 02/g	1.85	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.2	5 days (Bridie et al. 1979)
EC50 values to microorganisms, mg/l	10954 Microtox (Nacci et al. 1986)	
LC50 values to fishes, mg/l	> 5000	24hr, Carassius auratus (Bridie et al. 1979)

830 • Diethyleneglycol monomethylether 111-77-3

Synonyms	Diethylene glycol monomethyl ether 1-Methoxy-3-oxabutan-5-ol 2-(2-Methoxyethoxy)ethanol	
EC50 values to microorganism, mg/l	150688	Biodegradation inhibition (Vaishnav 1986)
LC50 values to fishes, mg/l	7500 > 5000	96hr, Lepomis macrochirus (Dawson et al. 1977) 24hr, Carassius auratus (Bridie et al. 1979)

831 • Diethylfumarate 623-91-6

LC50 values to fishes	4.2 4.5	96hr, Umbra pygmaea (Bender & Westmann 1976) 96hr, Pimephales promelas (Kemp et al. 1973)

D

832 • Diethylhexylphthalate 117-81-7

Synonyms	Phthalic acid, bis(2-ethylhexyl) ester Benzenedicarboxylic acid (bis(2-ethylhexyl) ester Bis(2-ethylhexyl)phthalate Di(2-ethylhexyl)orthophthalate Di(2-ethylhexyl)phthalate Benzene-1,2-dicarboxylic acid bis(2-ethylhexyl)ester	
Sumformula of the chemical	C24H3804	
Use	Plasticizer for many resins and elastomers.	
State and appearance	Light-coloured liquid.	
Odour	Odourless.	
Molecular weight	391	
Specific gravity (water=1)	0.9861	
Vapour pressure, mmHg	1.32	200 °C
Boiling point, °C	231	5 mm
Flashing point, °C	218	
Log octanol/water coefficient, log Pow	5.03 5.11	(Anon. 1986) (Anon. 1988)
Henry's law constant, Pa x m^3/mol	0.99	(Anon. 1988)
Mobility	Equilibrium distribution: air water solid	*mass %* 1.62 4.74 93.65 (Anon. 1988).
Other physicochemical properties	Insoluble in water; miscible with mineral oil. Combustible.	

Total degradation in water	Biodegradaation: 29% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Other information about degradation	Degradation of di-2-ethylhexyl-phthalate:

ENVIRONMENT	*INIT.CONC. mg/l*	*REDOX-COND.*	*TEMP. °C*	*DEGRADATION %/day*	*REF.*
water	5	aerobic	25	0/7	a
water	10	aerobic	25	0/7	a
water (adapted)	5	aerobic	25	95/7	a
water (adapted)	10	aerobic	25	93/7	a
freshwater	0.002	aerobic	29	35/40	b
freshwater	0.2	aerobic	29	62/40	b
riverwater	1	aerobic	room	63/35	c
freshwater sediment	1	aerobic	22	0/7	d
freshwater sediment	1	aerobic	22	59/30	d
freshwater sediment	1	aerobic	22	0/30	d
sludge	100	aerobic	30	48/20	e
soil	-	-	25–30	70/3	f
soil	0.00251	aerobic	20	0/14	g
soil (adapted)	0.00251	aerobic	20	0/28	g
soil	500	aerobic	30	92/30	h
soil	500	anaerobic	30	33/30	h
soil	2	aerobic	-	79-90/146	i
soil	20	aerobic	-	78-90/146	i

a) Tabak et al. 1981
b) Subba-Rao et al. 1982
c) Saeger & Tucker 1976
d) Johnson & Lulves 1975
e) Engelhardt et al. 1977
f) Yoshida et al. 1979
g) Hutchins & Ward 1984
h) Shanker et al. 1985
i) Fairbanks et al. 1985
(Anon. 1987b).

Bioconcentration factor, fishes	1.0–3.4 8w, Cyprinus carpio, conc 1 mg/l 1.3–29.7 8w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
LD50 values to mammals in oral exposure, mg/kg	26000 orl-gpg 143 orl-man 30000 orl-mus 30600 orl-rat 34000 orl-rbt (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	14000 ipr-mus 30700 ipr-rat 1060 ivn-mus 250 ivn-rat 10000 skn-gpg (Sweet 1987)

D

TDLo values to mammals in oral exposure, mg/kg	20000 16800 2040 6000 260000 216000	orl-gpg, 10d male, paternal eff. orl-mus, 7d male, paternal eff. orl-mus, 1-17d preg specific developmental abnormalities orl-rat, 10d male, paternal eff. orl-mus, 2Y-C, tumorigenic orl-rat, 2Y-C, tumorigenic (Sweet 1987)
TDLo values to mammals in non-oral exposure, mg/kg	25560 24000 5000 50 5 2970	ipr-mus, 1d male, eff. on fertility ipr-mus, 7-9d preg, eff. on fertility ipr-rat, 5-15d preg, effects on embryo or fetus ivn-mus, 1d preg, eff. on fertility ivn-mus, 8d preg, eff. on fertility scu-mus, 3d male, eff. on fertily effects on embryo or fetus (Sweet 1987)
Health effects	Skin and eye irritation data: skin, rbt, 500 mg, 24hr, mild; eye, rbt, 500 mg; eye, rbt, 500 mg, 24hr, mild (Sweet 1987).	
Carcinogenicity	NTP carcinogenesis bioassay (feed); clear evidence: mouse, rat (Sweet 1987).	
Mutagenicity	Mutation data: cytogenetic analysis: ham, orl. 7500 mg/kg; hmn, leukocyte, 6 mg/l; unscheduled DNA synthesis: rat, liver, 0.500 mmol/l; rat, orl, 670 mg/kg; dominant lethal test: mus, ipr, 12780 mg/kg; mus, scu, 2970 mg/kg, 10 D-l; gene conversion and mitotic recombination: S. cerevisiae, 5000 mg/l; microbial mutation without S9: S. cerevisiae, 1541 mg/l; microsomal assay: mus, lymphocyte, 40 mg/l; S. typhimurium, 5 mg/plate; oncogenic transformation: ham, orl, 750 mg/kg; ham, embryo, 4 mg/l; sex chromosome loss and nondisjunction: ham, liver, 50 mg/l; sperm morphology: rat, orl, 1 pph, 60 D-C (Sweet 1987).	
LC50 values to crustaceans, mg/l	> 300	96hr, 21 °C, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	> 3000	48hr, Oryzias latipes (MITI 1992)

833 • Diethylmaleate 141-05-9

LC50 values to fishes, mg/l	18	96hr, Pimephales promelas (Kemp et al. 1973)

834 • Diethylphthalate 84-66-2

Use	Solvent.
Molecular weight	222

Log octanol/water coefficient, log Pow	2.24	(Anon. 1988)
Henry's law constant, Pa x m³/mol	0.044	(Anon. 1988)
Mobility	Equilibrium distribution:	
		mass %
	air	1.50
	water	95.94
	solid	2.55
		(Anon. 1988).
LC50 values to algae, mg/l	24–33	96hr, Gymnodinium breve (Wilson et al. 1978)
LC50 values to crustaceans, mg/l	52	48hr, Daphnia magna (LeBlanc 1980)
LC50 values to fishes, mg/l	110	96hr, Lepomis macrochirus (Buccafusco et al. 1981)
	30	96hr, Cyprinodon variegatus (Heitmuller et al. 1981)

835 • Diethylsuccinate

123-25-1

LC50 values to fishes, mg/l	140	96hr, Pimephales promelas (Kemp et al. 1973)

836 • 1,3-Diethylthiourea

105-55-5

Other information about mammals	ALD = 62.0–94.0 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987).

837 • Difenacoum

56073-07-5

Synonyms	3-(3-p-Diphenyl-1,2,3,4-tetrahydronaphth-1-yl)-4-hydroxycoumarin
Sumformula of the chemical	$C_{31}H_{24}O_3$
Products containing the chemical	Ratak-jauhe * difenacoum 1 g/kg Ratak-syötti * difenacoum 0.05 g/kg (PESREG)
Use	Active ingredient in rodenticides.
Instructions for handling	Stable at least for 6 months (50 °C, 25 °C and 37 °C). (PESREG)
State and appearance	Solid, white powder. (PESREG)
Odour	Odourless.
Molecular weight	444
Specific gravity (water=1)	1.25
Vapour pressure, mmHg	0.000012 45 °C 0.000058 55 °C (PESREG)
Melting point, °C	215–217 °C (PESREG)
Mobility	In the soil column studies difenacoum (1.3 kg a.i./ha) wasn't found (analysis unit 0.006 mg/l) in the leachate of three soil samples after two days rainfall (200 ml). (PESREG)

Other physicochemical properties	Insoluble in water. (PESREG) Soluble in benzene, in chloroform and in other chloronated solvents. Solubility in organic solvents (mg/100 ml): ethylacetate: 0.2 acetone 0.5 chloroform 2.5 (PESREG)
LD50 values to mammals in oral exposure, mg/kg	1.11–2.21 orl-rat female (PESREG) 1.8 orl-rat male (PESREG) 0.8 orl-mus (PESREG) 2 orl-rbt male (PESREG) 50 orl-dog (PESREG) 100 orl-cat (PESREG) 80–100 orl-big (PESREG)
LD50 values to mammals in non-oral exposure, mg/kg	2.5–5.0 24hr, idr-rat female PESREG
LD50 values to birds in oral exposure, mg/kg	66 16d, Coturnix virginianus PESREG
Subacute LC50 values to birds in feeding exposure, mg/kg	6.3–56.7 5d, Anas platyrhyncos (PESREG)
Effects on invertebrates	LD50, > 1000 mg/kg, 24hr, Musca domestica LD50, > 2500 mg/kg, 24hr, Tribolium castaneum LD50, > 1000 mg/kg, 24hr, Blattella germanica (PESREG)
LC50 values to fishes, mg/l	0.41 24hr, Salmo gairdneri 0.28 48hr, Salmo gairdneri 0.1 96hr, Salmo gairdneri (PESREG)

838 • Difenzoquat 49866-87-7

Synonyms	1,2-Dimethyl-3,5-diphenyl-1-H-pyrazolium Difenzoquat methyl sulfate 1,2-Dimethyl-3,5-diphenyl-1-H-pyrazolium methyl sulfate (CAS 43222-48-6)
Use	Active ingredient in herbicides.
LC50 values to fishes, mg/l	696 96hr, Lepomis macrochirus 694 96hr, Salmo gairdneri (Pesticide Manual 1983)

839 • Difolatan 2425-06-1

Use	Fungicide.
LC50 values to crustaceans, mg/l	0.8 96hr, Gammarus lacustris (Sanders 1969)
Other information about water organisms	LC50 0.04 mg/l, 96hr, Pteronarcys californica (Sanders & Cope 1968)

840 • Diheptyl phthalate

3648-21-3

Synonyms	Benzene-1,2-dicarboxylic acid diheptyl
Boiling point, °C	212 5 mmHg (MITI 1992)
Total degradation in water	Biodegradation: 36% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
Bioconcentration factor, fishes	0.9–2.2 8w, Cyprinus carpio, conc 1 mg/l 6.2–16.7 8w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	2000–3000 48hr, Oryzias latipes (MITI 1992)

841• 9,10-Dihydro-8a,10-diazonia-phenanthrene dibromide

85-00-7

Synonyms	Diquat Diquat dibromide 1,1'-Ethylene-2,2'-bipyridyliumdibromide Reglon Reglone Reglox Preeglone
Sumformula of the chemical	C12H12N2Br2
Use	Active ingredient in herbicides.
Molecular weight	344.08
Vapour pressure, mmHg	0.000000075 (KEMI 1991)
Water solubility, mg/l	700000 20 °C (KEMI 1991) 700000 (MITI 1992)
Mobility	Diquat is absorbed tightly to clay mineral. Mobility is very low but it depends on soil type. Mobility increases when clay in soil decreases. Koc: 205–691, Rf: 0.00–0.09 (KEMI 1991).
Photochemical degradation in air	Photolysis half-lives in water and air are from some days to some weeks under Swedish climate conditions. Photolysis products are first 1,2,3,4-tetrahydro-1-oxo-pyrido(1,2-α)-5-pyrazinium salt and then picoline amide and picolinic acid (KEMI 1991).
Hydrolysis in water	Diquat is hydrolytic stabile at acidic and neutral pH; at basic pH transformation is happening (KEMI 1991).
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

Other information about degradation	When diquat and its degradationproducts are bounded to clay, degradation is in those cases very slow. Microorganisms can also decompose diquat. Degradation is extremely slow, half-life can be tens of years (KEMI 1991).
Bioconcentration factor, fishes	< 0.6–1.4 6w, Cyprinus carpio, conc 1 mg/l < 5.7 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	120 orl-rat 231 orl-rat 233 orl-mus 188 orl-gpg (Lewis & Sweet 1984) 37 orl-cows (Verschueren 1983) 120–190 orl-rat (KEMI 1991)
LD50 values to mammals in non-oral exposure, mg/kg	> 750 skn-rbt (Verschueren 1983) 20 scu-rat 400 unk-man (Lewis & Sweet 1984) 400 idr-mus, idr-rbt (KEMI 1991) 650 idr-rat (KEMI 1991)
LC50 values to mammals in inhalation exposure, mg/m^3	35 ihl-rat (KEMI 1991)
LDLo values to mammals in oral exposure, mg/kg	187 orl-dog 56 orl-ctl (Lewis & Sweet 1984)
LDLo values to mammals in non-oral exposure, mg/kg	500 ipr-rat 14 ivn-rat (Lewis & Sweet 1984)
TDLo values to mammals in non-oral exposure, mg/kg	7 ivn-rat, 6d preg. (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	564 orl-dck (Lewis & Sweet 1984) 200–400 orl-ckn (KEMI 1991)
LDLo values to birds in oral exposure, mg/kg	373 orl-ckn (Lewis & Sweet 1984)
Effects on amphibia	LC50, 48hr, 40 mg/l, Bufo bufo (KEMI 1991)
Effects on bees	LD50, 24hr, 0.081 mg/bee (KEMI 1991)
Effects on plants	Beans (Phaseolus vulgaris) were sprayed to 'run off' at the fully expanded primary leaf stage. Diquat at 0.001 M increased leaf-cell membrane permeability after exposure for 12hr or less (Prendeville & Warren 1977).
EC50 values to algae, mg/l	0.011 96hr, Selenastrum capricornutum (KEMI 1991)
LOEC values to algae, mg/l	15 rpd, schr, Phaedactylum tricornutum (Walsh 1972) 15 rpd, schr, Isochyris galbana (Walsh 1972)
NOEC values to algae, mg/l	0.0068 Selenastrum capricornutum (KEMI 1991)
LC50 values to crustaceans, mg/l	7.1 act, Daphnia magna (Kenaga 1979) 0.048 96hr, Hyalella azteca (Wilson & Bond 1969) 7.1 24hr, Daphnia magna (Crosby & Tucker 1966) 7.1 48hr, Daphnia magna (KEMI 1991) 0.048 Hyallella (KEMI 1991) 40 72hr, crab (KEMI 1991)

LC50 values to fishes, mg/l	> 10	act, Salmo gairdneri (Kenaga 1979)
	2.1	96hr, Stizostedion vitreum
	16	48hr, Esox lucius
	2.1	96hr, Catostomus commersoni (Gilderhus 1967)
	7.8	96hr, Micropterus salmoides (Surber & Pickering 1962)
	289	96hr, Gambusia affinis (Leung et al. 1983)
	50	96hr, Cyprinus carpio (Chin & Sudderuddin 1979)
	30	96hr, Oncorhynchus kisutch
	19	144hr, Oncorhynchus kisutch (Lorz et al. 1979)
	90	24hr, Salmo gairdneri (Alabaster 1969)
	37	48hr, Rasbora heteromorpha
	70	48hr,hrd, Salmo gairdneri
	27	48hr, sfd, Salmo gairdneri (Kemp et al. 1973)
	2	96hr, Stizostedion lucioperca
	16	96hr, Esox lucius
	300	96hr, Salmo salar (KEMI 1991)
	48.5	48hr, Oryzias latipes (MITI 1992)
Other information about water organisms	LC50	48hr, 10 mg/l, mussel (KEMI 1991)

842 • Dihydroheptachlor

33360-84-8

Use	Insecticide.	
LC50 values to fishes, mg/l	0.044	96hr, Rasbora heteromorpha (Tooby et al. 1975)

843 • Diisobutyl phthalate

84-69-5

Use	Plasticizer.	
State and appearance	Liquid.	
Specific gravity (water=1)	1.04	20/20 °C
Boiling point, °C	327	
Flashing point, °C	196	
LC50 values to crustaceans, mg/l	3	96hr, 21 °C, Nitocra spinipes (Linden et al. 1979)

844 • Diisobutylketone

108-83-8

Use	Solvent.
Odour	Quality: sweet, ester Hedonic tone: pleasant Threshold odour concentration absolute: < 0.11 ppm 50% recognition: 0.31 ppm 100% recognition: 0.31 ppm Odour index 100% recognition: 4 258 (Hellman & Small 1974).

Water solubility, mg/l	500 20 °C
Boiling point, °C	168
Volatilization	Relative volatility (nBuAc=1) = 0.17
LD50 values to mammals in oral exposure, mg/kg	1416 orl-mus

845 • Diisodecyl phthalate 26761-40-0

Synonyms	Benzene-1,2-dicarboxylicacid diisodecyl
Boiling point, °C	420 (MITI 1992)
Total degradation in water	Biodegradation: 42% by BOD (on the upward trend) period: 21d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
Bioconcentration factor, fishes	< 3.6 8w, Cyprinus carpio, conc 1 mg/l < 14.4 8w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	> 3000 48hr, Oryzias latipes (MITI 1992)

846 • Diisononylphthalate 28553-12-0

LC50 values to fishes, mg/l	0.42 4 days, Ictalurus punctatus (Birge et al. 1978)

847 • Diisopentyl ether 544-01-4

Water solubility, mg/l	10.8 (MITI 1992)
Boiling point, °C	172.5–173 (MITI 1992)
Log octanol/water coefficient, log Pow	4.25 (MITI 1992)
Total degradation in water	Biodegradation: 8% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	117–313 8w, Cyprinus carpio, conc 60 000 mg/l 84–260 8w, Cyprinus carpio, conc 6000 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	4.7 48hr, Oryzias latipes (MITI 1992)

848 • Diisophorone hydrazone 42398-17-4

Other information about mammals	LDfr = 50.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

849 • Diisopropanol amine 110-97-4

Synonyms	Bis(2-hydroxypropyl)amine	
Chemical oxygen demand, g 02/g	1.9	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.02	5 days (Bridie et al. 1979)
LC50 values to fishes, mg/l	> 5000	24hr, Carassius auratus (Bridie et al. 1979)

850 • Diisopropyl amine 108-18-9

Odour	Quality: fishy, amine, ammoniacal Hedonic tone: unpleasant to pleasant Threshold odour concentration absolute: 0.13 ppm 50% recognition: 0.38 ppm 100% recognition: 0.85 ppm Odour index 100% recognition: 92 823 (Hellman & Small 1974).	
EC50 values to algae, mg/l	20	96hr, rpd, Selenastrum capricornutum (Calamari et al. 1982)
LC50 values to crustaceans, mg/l	448 187	48hr, Daphnia magna (Hermens et al.1984) 24hr, Daphnia magna (Calamari et al.1982)
EC50 values to crustaceans, mg/l	60	16 days, rpd, Daphnia magna (Hermens et al. 1984)
LC50 values to fishes, mg/l	37	96hr, Salmo gairdneri (Calamari et al. 1980)

851 • Diisopropyl naphthalene 38640-62-9

Melting point, °C	300	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).	
Bioconcentration factor, fishes	1310–3930 370–3860	8w, Cyprinus carpio, conc 0.05 mg/l 8w, Cyprinus carpio, conc 0.005 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be accumulated on a medium level (Anon. 1987).	
LC50 values to fishes, mg/l	4.5	48hr, Oryzias latipes (MITI 1992)

D

852 • Diisopropylbenzene, m-(60%) and p-(40%)

25321-09-9

Sumformula of the chemical	C12H18	
Water solubility, mg/l	0.072 0.0405	m- (MITI 1992) p- (MITI 1992)
Boiling point, °C	202	m- (MITI 1992)
Log octanol/water coefficient, log Pow	5.13 5.23	m- (MITI 1992) p- (MITI 1992)
Total degradation in water	Biodegradaation: 0% by BOD period: 14d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).	
Bioconcentration factor, fishes	503–1680 530–2300 546–3210 512–2960	m-, 8w, Cyprinus carpio, conc 0.02 mg/l p-, 8w, Cyprinus carpio, conc 0.02 mg/l m-, 8w, Cyprinus carpio, conc 0.002 mg/l p-, 8w, Cyprinus carpio, conc 0.002 mg/l (MITI 1992)
LC50 values to fishes, mg/l	2.6	48hr, Oryzias latipes (MITI 1992)

853 • Diisopropylether

108-20-3

Synonyms	Isopropyl ether	
Sumformula of the chemical	C6H14O	
Use	Solvent.	
Odour	Quality: sweet Hedonic tone: pleasant Threshold odour concentration absolute: 0.017 ppm 50% recognition: 0.053 ppm 100% recognition: 0.053 ppm Odour index 100% recognition: 2 924 528 (Hellman & Small 1974).	
Boiling point, °C	68–69	
Log octanol/water coefficient, log Pow	1.52	(Sangster 1989)
Henry's law constant, Pa x m³/mol	175.7	calc. (Yaws et al. 1991)
LC50 values to fishes, mg/l	7000 6600 380 91.7	96hr, Lepomis macrochirus 96hr, Menidia audens (Dawson et al. 1977) 24hr, Carassius auratus (Bridie et al. 1979) 96hr, Pimephales promelas (Veith et al. 1983)

854 • Diketene

674-82-8

Sumformula of the chemical	C4H4O2	
Melting point, °C	-6.5	(MITI 1992)

Boiling point, °C	127.4 (MITI 1992)
Total degradation in water	Biodegradation: 95–102% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

855 • Dilauryl-thio dipropionic ester 123-28-4

Synonyms	Dilauryl thiodi ester propionate
Melting point, °C	39–44 (MITI 1992)
Total degradation in water	Biodegradation: 82% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

856 • 2,3-Dimercapto-1-propanol 59-52-9

Synonyms	2,3-Dimercaptopropanol
Effects on plants	10-4 mol/l (6 hours) —increase in rate of C-mitosis of Allium cepa roots (Ramel 1969).

857 • Dimethoxane 828-00-2

Synonyms	2,6-Dimethyl-1,3-dioxane-4-yl-acetate Acetic acid, ester with 2,6-dimethyl-m-dioxan-4-ol Acetic acid, 2,6-dimethyl-m-dioxan-4-yl ester Acetomethoxane 6-Acetoxy-2,4-dimethyl-m-dioxane DDOA 2,6-Dimethyl-m-dioxan-4-ol acetate
Sumformula of the chemical	C8H14O4
Use	Microbicide.
Molecular weight	174.22
Boiling point, °C	68–72, 4 mmHg (MITI 1992)
Total degradation in water	Biodegradation: 76–83% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	1930 orl-rat (Sweet 1987)

TDLo values to mammals in oral exposure, mg/kg	948000 orl-rat, tumorigenic (Sweet 1987)
Mutagenicity	Mutation data: microsomal assay: S. typhimurium, 5.5 mg/plate; sex chromosome loss and nondisjunction: D. melanogaster, parental, 1 pph (Sweet 1987).
LD50 values to birds in oral exposure, mg/kg	> 98 orl-Agelaius phoeniceus (Schafer et al. 1983)
LC50 values to fishes, mg/l	44 96hr, Rasbora heteromorpha (Tooby et al. 1975)

858 • Dimethoxon 1113-02-6

Other information about mammals	LDfr = 75.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

859 • 4,4-Dimethoxy diphenylamine 101-70-2

Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987) (4,4'-dimethoxy diphenyl amine).

860 • p-Dimethoxybenzene 150-78-7

LC50 values to fishes, mg/l	117 96hr, Pimephales promelas (Veith et al. 1983)

861 • 2,6-Dimethoxytoluene 5673-07-4

LC50 values to fishes, mg/l	20.5 96hr, Pimephales promelas (Veith et al. 1983) 20.2 96hr, Pimephales promelas (Broderius & Kahl 1985)

862 • Dimethyl amine 124-40-3

Sumformula of the chemical	C2H7N
Melting point, °C	-37 (MITI 1992)
Boiling point, °C	52 (MITI 1992)
Log octanol/water coefficient, log Pow	-0.38 (Sangster 1989)
Aerobic degradation in sediment	Biodegradation: 51% by BOD (on the upward trend) period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
EC50 values to algae, mg/l	9 rpd, schr, 96hr, Selenastrum capricornutum (Calamari et al. 1982b) 30 rpd, act, 96hr, Chlorella pyrenoidosa (Leeuwen et al. 1985)

LC50 values to crustaceans, mg/l	48 50	24hr, Daphnia magna (Calamari et al. 1982b) 48hr, Daphnia magna (Leeuwen et al. 1985)
LC50 values to fishes, mg/l	17 118 1.2 210	sfd, 96hr, Salmo gairdneri (Calamari et al. 1980) hrd, 96hr, Salmo gairdneri (Calamari et al. 1980) 50d, Salmo gairdneri (Calamari et al. 1979) 96hr, Poecilia reticulata (Leeuwen et al. 1985)

863 • N, N-Dimethyl ethanolamine 108-01-0

Melting point, °C	-59 (MITI 1992)
Boiling point, °C	134.6 (MITI 1992)
Total degradation in water	Biodegradation: 60.5% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

864 • Dimethyl maleate 624-48-6

Sumformula of the chemical	C6H8O4
Water solubility, mg/l	79000 (MITI 1992)
Melting point, °C	< -10 (MITI 1992)
Boiling point, °C	205–207 (MITI 1992)
Total degradation in water	Biodegradation: 50–72% by BOD (on the upward trend) period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

865 • 2,3-Dimethyl naphthalene 581-40-8

Sumformula of the chemical	C12H12
Water solubility, mg/l	< 10 (MITI 1992)
Melting point, °C	101–102.5 (MITI 1992)
Boiling point, °C	269.2 (MITI 1992)
Total degradation in water	Biodegradation: 0–89% by BOD (on the upward trend) period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

866 • 2,6-Dimethyl naphthalene 581-42-0

Sumformula of the chemical	C12H12	
Log octanol/water coefficient, log Pow	4.31	(Sangster 1989)
Henry's law constant, Pa x m^3/mol	121.1	calc. (Yaws et al. 1991)

867 • 2,6-Dimethyl piperidine 504-03-0

Water solubility, mg/l	> 50000	(MITI 1992)
Boiling point, °C	127–128	(MITI 1992)
Total degradation in water	Biodegradation: 0–4% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.5 < 5.0	6w, Cyprinus carpio, conc 1 mg/l 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	30	48hr, Oryzias latipes (MITI 1992)

868 • O,O-Dimethyl S-(1-carboethoxybenzyl) dithiophosphate 2597-03-7

Synonyms	Fenthoate Bay 33051 Bayer 18510 Cidemul Cidial Elsan S-α-Ethoxycarbonylbenzyl 0,0-dimethylphosphorodithioate Phenthoate 0,0-Dimethyl-S-(1-ethoxycarbonyl-1-phenyl) methylphosphorodithioate	
Sumformula of the chemical	C12H17O4PS2	
Use	Insecticide.	
Molecular weight	320.38	
Water solubility, mg/l	1	(MITI 1992)
Melting point, °C	16–17	(MITI 1992)
Boiling point, °C	186–187, 5 mmHg	(MITI 1992)
Log octanol/water coefficient, log Pow	3.41	(MITI 1992)

Total degradation in water	Biodegradation: 0–3% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992)	
Bioconcentration factor, fishes	3.7–29 7.1–34	6w, Cyprinus carpio, conc 0.0025 mg/l 6w, Cyprinus carpio, conc 0.00025 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non–accumulative or low accumulative (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	200 72 150 500 400	orl-rat orl-rbt orl-mus orl-dog orl-gpg (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	700 2620	skn-rat skn-mus (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	36.6 300 218	orl-ckn orl-qal orl-brd (Lewis & Sweet 1984)
LC50 values to crustaceans, mg/l	0.002	Daphnia pulex (Nishiuchi & Hashimoto 1967)
LC50 values to fishes, mg/l	0.84 2.9 2.5 2 1	24hr, Cyprinus carpio (Hashimoto et al. 1982) 96hr, Carassius auratus 96hr, Phoxinus phoxinus (Pesticide Manual 1983) 48hr, Cyprinus carpio (Nishiuchi & Hashimoto 1967) 48hr, Oryzias latipes (MITI 1992)

869 • O,O-Dimethyl S-(2(methylamino)-2-oxoehyl) phosphorodithioate

60-51-5

Synonyms	0,0-Dimethyl-S-(N-methylcarbamoyl)-methyl)phosphorodithioate 0,0-Dimethyl-S-(N-methylcarbamoylmethyl) dithiophosphate Dimethoate Acetic acid,0,0-dimethyldithiophosphoryl-N-monomethylamide salt 0,0-Dimethyldithiophosphoryl acetic acid N-monomethylamidesalt Dimeton Fosfamid Fosfotox Phosphamide Rogon Trimetion Phosphorodithioic acid, 0,0-dimethylester, s-ester with 2-mercapto-N-methylacetamide
Sumformula of the chemical	C5H12NO3PS2

Use	Acaricide, active ingredient in insecticides.
Molecular weight	229.27
Vapour pressure, mmHg	0.0000083 at 25 °C (KEMI 1991)
Water solubility, mg/l	25000 room temp. 25000 at 21 °C (KEMI 1991) > 1% (MITI 1992)
Melting point, °C	51–52 (KEMI 1991) 48–50 (MITI 1992)
Log octanol/water coefficient, log Pow	1.78 (Anon. 1988) 0.7 (KEMI 1991) 0.79 (MITI 1992)
Log soil sorption coefficient, log Kom	0.72 (Sabljic 1987)
Henry's law constant, Pa x m³/mol	0.00001 (Anon. 1988)
Mobility	Equilibrium distribution: *mass %* air 0.00 water 99.08 solid 0.91 (Anon. 1988) The leaching behaviour of dimethionate was studied with soil thin-layer plates and with soil columns. According to the studies dimethionate is very mobile. Rf: 0.89–0.97 (sandy loam – loam) Koc: 12–35 (sandy soil – clay soil) (KEMI 1991)
Photochemical degradation in air	Photolysis half-lives are 7–16 days in TLC-experiment. Major photoproducts are dimethylphosphor acid and O-methoate. (KEMI 1991)
Hydrolysis in water	Dimethionate is hydrolysis stabile at neutral and basic conditions. (KEMI 1991)
Aerobic degradation in soil	Dimethionate is degraded in soil by microorganisms. Degradation product at aerobic and anaerobic conditions is O-desmethyl-dimethoate. Half-life in aerobic degradation varies from 3–42 days and 9–27% of C-14 applied radioactivity was recovered after 6 months (KEMI 1991)
Total degradation in water	50% of original compound found after 8 weeks (river water, initial conc. 0.010 mg/l) (Verschueren 1983) Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992)
Bioconcentration factor, fishes	0.4–0.8 6w, Cyprinus carpio, conc 2 mg/l < 1.6 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987) (O,O-dimethyl-S-(N-methyl carbamoyl methyl) dithiophosphate).
LD50 values to mammals in oral exposure, mg/kg	152 orl-rat 60 orl-mus 30 orl-hmn 15 orl-mam 400 orl-dog (Lewis & Sweet 1984)

LD50 values to mammals in non-oral exposure, mg/kg	45 60 353 100 350 450	ipr-mus scu-mus skn-rat ipr-rat scu-rat ivn-rat (Lewis & Sweet 1984)
LDLo values to mammals in oral exposure, mg/kg	300	orl-cat (Lewis & Sweet 1984)
TDLo values to mammals in oral exposure, mg/kg	256 120	orl-rat orl-rat (Lewis & Sweet 1984)
TDLo values to mammals in non-oral exposure, mg/kg	176	ims-rat (Lewis & Sweet 1984)
Carcinogenicity	NCI carcinogenesis bioassay completed: results negative, mus, rat (Lewis & Sweet 1984).	
LD50 values to birds in oral exposure, mg/kg	22 7 37	orl-brd orl-bwd orl-ckn (Lewis & Sweet 1984)
	6.6–17.8 31.6	orl-Agelaius phoenicus, orl-Sturnus vulgaris (Schafer et al. 1983)
Effects on amphibia	LC50 0.008 mg/l, 96hr, tadpoles of Rana hexadactyla (Khangarot et al. 1985). NOEC, 1 mg/l, 100d, Xenopus laevis, mortality. NOEC, 32 mg/l, 100d, Xenopus laevis, development. NOEC, 32 mg/l, 100d, Xenopus laevis, growth. (Slooff & Canton 1983)	
Effects on arthropods	NOEC, 0.32 mg/l, 25d, Culex pipiens, mortality. NOEC, 0.32 mg/l, 25d, Culex pipiens, development. (Slooff & Canton 1983)	
Effects on plants	NOEC, 32 mg/l, 7d, Lemna minor, specific growth rate (Slooff & Canton 1983)	
Effects on microorganisms	NOEC, 320 mg/l, 0,3d, Pseudomonas fluorescens, specific growth rate. NOEC, 32 mg/l, 4d, Microcystis aeruginosa, specific growth rate. (Slooff & Canton 1983)	
NOEC values to algae, mg/l	32	96hr, grw, Microcystis aeruginosa (Slooff & Canton 1983)
	100	4d, grw (biomass), Scendesmus pannonicus (Slooff & Canton 1983)
LC50 values to crustaceans, mg/l	0.01	Daphnia magna (Nishiuchi & Hashimoto 1967)
	0.001	48hr, Crangon crangon (Kemp et al. 1973)
	4.57	96hr, Saccobranchus fossilis (Verma et al. 1982a)
	6.4	48hr, Daphnia magna (Hermens et al. 1984)
	2.5	act, Daphnia magna (Kenaga 1979)
	4.275 2.63	1d, Macrobrachium lamarrei 3d, Macrobrachium lamarrei (Mary et al. 1986)
EC50 values to crustaceans, mg/l	0.31	16 days, rpd, Daphnia magna (Hermens et al. 1984)
NOEC values to crustaceans, mg/l	0.032	21 days, srv, Daphnia magna (Slooff & Canton 1983)
	0.1	21d, rpd, Daphnia magna (Slooff & Canton 1983)

D

LC50 values to fishes, mg/l	8.5 act, Salmo gairdneri 6 act, Lepomis macrochirus (Kenaga 1979) 28 24hr, Poecilia reticulata 20 24hr, Salmo gairdneri (Edwards 1977) 18.97 96hr, Poecilia reticulata (Gupta et al. 1984) 40–60 96hr, Gambusia affinis (Pesticide Manual 1983) > 40 48hr, Cyprinus carpio (Nishiuchi & Hashimoto 1967) 4.65 4d, Cyprinus carpio (Kulshrestha & Arora 1986) 840 48hr, Oryzias latipes (MITI 1992)
NOEC values to fishes, mg/l	32 28d, srv, Poecilia reticulata 0.1 28d, srv + bhv, Poecilia reticulata 10 28d, grw, Poecilia reticulata 0.32 40d, srv, Oryzias latipes 0.32 40d, srv + bhv, Oryzias latipes 100 40d, grw, Oryzias lapites (Slooff & Canton 1983)
Effects on the physiology of water organisms	Biochemical effect (change in physiochemical process including glycogen uptake, cholesterol levels and lipid analysis): 0.41 mg/l, 35 d, Channa punctatus, Labeo rohita, Tilapia mossambica (Ghosh 1987).
Other information about water organisms	NOEC, 100 mg/l, 21d, Hydra oligactis, specific growth rate. NOEC, 32 mg/l, 40d, Lymnaea stagnalis, mortality. NOEC, 10 mg/l, 40d, Lymnaea stagnalis, reproduction. NOEC, 32 mg/l, 40d, Lymnaea stagnalis, hatching. (Slooff & Canton 1983)

870 • Dimethyl sulfate 77-78-1

Sumformula of the chemical	C2H6O4S
Molecular weight	126.14
Health effects	Skin and eye irritation data: Skin, rabbit: 10 mg, 24hr, open, severe; eye, rabbit; 100 mg, 4 s, rinse, severe; eye, rabbit, 0.05 mg, 24hr, severe (Sweet 1987).
Carcinogenicity	Carcinogenic (Anon. 1974).
LC50 values to fishes, mg/l	7.5 96hr, Lepomis macrochirus 15 96hr, Menidia audens (Dawson et al. 1977)

871 • Dimethyl sulfoxide 67-68-5

Synonyms	DMSO
Sumformula of the chemical	C2H6OS
Use	Solvent.
Boiling point, °C	189
Log octanol/water coefficient, log Pow	-1.35 (Sangster 1989)

Volatilization	Relative volatility (nBuAc=1) = 0.04
Total degradation in water	Biodegradation: 3.1% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.4 6w, Cyprinus carpio, conc 1 mg/l < 4 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	21000 orl-mus
LD50 values to birds in oral exposure, mg/kg	100 orl-Agelaius phoeniceus 100 orl-Sturnus vulgaris (Schafer et al. 1983)
EC50 values to microorganisms, mg/l	12038 INT (Dutton et al. 1986) 87900 Microtox (Tarkpea et al. 1986)
LC50 values to fishes, mg/l	33000 48hr, Oryzias latipes (MITI 1992)

872 • 2,2-Dimethyl-1,3-propanediol 126-30-7

Melting point, °C	129.5 (MITI 1992)
Boiling point, °C	211.1 (MITI 1992)
Total degradation in water	Biodegradation: 1% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Bioconcentration factor, fishes	0.3–0.5 6w, Cyprinus carpio, conc 10 mg/l < 9 6w, Cyprinus carpio, conc 1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon.1987) (2,2'-dimethyl-1,3-propanediol).
LC50 values to fishes, mg/l	> 10 000 48hr, Oryzias latipes (MITI 1992)

873 • N, N-Dimethyl-2,2-diphenylacetamide 957-51-7

Synonyms	N, N-Dimethyl-α-phenyl-benzeneacetamide Diamide N, N-Dimethyldiphenylacetamide N, N-α, α-Diphenylacetamide Diphenamide 2,2-Diphenyl-N,N-dimethylacetamide Diphenylamide Fenam
Sumformula of the chemical	C16H17NO

Use	Herbicide.
Molecular weight	239.34
LD50 values to mammals in oral exposure, mg/kg	1000 orl-dog 1000 orl-mnk 600 orl-mus 685 orl-rbt (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	500 ipr-mus 800 scu-mus (Sweet 1987)
Mutagenicity	Mutation data: cytogenetic analysis: mus – unreported route, 10 mg/kg (Sweet 1987).
Effects on plants	Germinated seedlings of barley (Hordeum vulgare) were grown in diphenamid-treated silica sand: 0.5 ppm diphenamid (in mg active material per litre solution; 12 ml of the solution was added to 225 g dry sand) caused 50% root inhibition over 72 h (O'Sullivan & Prendeville 1974).
LC50 values to crustaceans, mg/l	56 48hr, Daphnia magna 50 48hr, Cypridopsis vidua (Sanders 1970)

874 • 1,5-Dimethyl-2,4-dinitrobenzene

EC50 values to crustaceans, mg/l	24.3	mbt, 48hr, Daphnia magna (Pearson et al. 1979)
LC50 values to fishes, mg/l	7.9	96hr, Pimephales promelas (Pearson et al. 1979)

875 • 3,3-Dimethyl-2-butanone 75-97-8

LC50 values to fishes, mg/l	87	96hr, Pimephales promelas (Veith et al. 1983)

876 • 4,5-Dimethyl-2-nitroaniline 6972-71-0

Other information about water organisms	EC50 (60hr) 52 mg/l, rpd, Tetrahymena pyriformis (Schultz & Applehans 1985).

877 • 0,0-Dimethyl-s-(2-ethyl-mercaptoethyl) dithiphosphate 640-15-3

Synonyms	Thiometon Morphothion Ekatin Thiameton
Sumformula of the chemical	C6H1502PS3
Use	Insecticide, acaricide.
Molecular weight	246.36

LD50 values to mammals in oral exposure, mg/kg	25 60	orl-rat orl-mus (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	179 30 34	skn-mus ipr-rat ipr-mus (Lewis & Sweet 1984)
LC50 values to crustaceans, mg/l	11	96hr, Saccobranchus fossilis (Verma et al. 1978)
LC50 values to fishes, mg/l	3.2	96hr, Rasbora heteromorpha (Tooby et al. 1975)

878 • N, N-Dimethylacetamide 127-19-5

Synonyms	Acetamide, N, N-dimethyl-	
Sumformula of the chemical	C4H9NO	
EINECS-number	2048264	
Water solubility, mg/l	> 100000(MITI 1992)	
Melting point, °C	< -10	(MITI 1992)
Boiling point, °C	165.5	754 mmHg (MITI 1992)
Total degradation in water	Biodegradation: 77–83% by BOD period: 14d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).	

879 •4-(Dimethylamine)-3,5-xylyl N-methylcarbamate 315-18-4

Synonyms	Mexacarbate Zectran Dowco 139 4-(Dimethylamino)-3,5-dimethylphenol–N-methylcarbamate Methyl carbamic acid, 4-(dimethylamino)-3,5-xylyl ester	
Sumformula of the chemical	C12H18N2O2	
Use	Herbicide, insecticide; pesticide for control of snails and slugs.	
Molecular weight	222.32	
Specific gravity (water=1)	> 1	
Vapour pressure, mmHg	< 0.1	139 °C
Water solubility, mg/l	100	25 °C
Melting point, °C	85	
Other physico-chemical properties	Flammability: combustible solid. Boiling characteristics: decomposes. Practically insoluble in water.	

Other information about degradation	In water with low pH, significant levels of this insecticide may persist for many weeks. In soil, 70% to 100% is degraded within the first 2 weeks by soil microorganisms (Sax 1986). Mexacarbate has a high rate of leaching in sandy soil. – It is also readily metabolized by soil microorganisms (Sax 1986).
Bioconcentration factor, fishes	45 (Verschueren 1983)
Bioconcentration factor, crustaceans	18 (Verschueren 1983)
Bioconcentration factor, other organisms	0–8 (Verschueren 1983)
Other information about bioaccumulation	In aquatic systems, mexacarbate will accumulate in algae, daphnia, and fish (Sax 1986). Food chain contamination potential moderate. Mexacarbate will accumulate in aquatic invertebrates and fish, but not to a great extent (Sax 1986).
LD50 values to mammals in oral exposure, mg/kg	14 orl-rat 15 orl-mus, orl-dom 15 orl-dog 37 orl-rbt 15 orl-gpg 16 orl-mam (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	1500 skn-rat, 15 ipr-mus 15 ipr-rat (Lewis & Sweet 1984)
LDLo values to mammals in non-oral exposure, mg/kg	15 ipr-mus (Sax 1986)
TDLo values to mammals in oral exposure, mg/kg	1200 orl-mus (Lewis & Sweet 1984) 1200 orl-mus, 78W-I, tumorigenic (Sax 1986)
TDLo values to mammals in non-oral exposure, mg/kg	90 scu-mus, 6-14d preg, teratogenic (Sax 1986)
Health effects	Acute poisoning from inhalation or skin absorption produces headache, weakness, dizziness, anxiety, tremors of the tongue and eyelids, and impairment of visual acuity. Prolonged contact may result in salivation, tearing, abdominal cramps, vomiting, sweating, and muscular fasciculations. Death can occur from respiratory difficulty, cyanosis, and convulsions (Sax 1986). This material is extremely toxic to humans; between 7 drops and 1 teaspoon may be lethal (Sax 1986). Extremely toxic by ingestion and a suspected carcinogen (Sax 1986).
Carcinogenicity	NCI carcinogenesis bioassay completed: results negative; mus rat (Lewis & Sweet 1984). Mexacarbate had a carcinogenic effect when applied orally to mice for 78 weeks (Sax 1986).

LD50 values to birds in oral exposure, mg/kg	4	orl-ckn
	3.21	orl-qal
	3	orl-dck
	10	orl-bwd
		(Lewis & Sweet 1984)
	6.47	orl-pgn
	1	orl-bwd
		(Sax 1986)
	10.0–13.3	orl-Agelaius phoeniceus
	23.7–31.6	orl-Sturnus vulgaris
	2.37	orl-Coturnix coturnix
	7.5	orl-Passer domesticus
	7.5	orl-Quiscalus quiscula
	5.62	orl-Columba livia
		(Schafer et al. 1983)
Effects on amphibia	283 mg/l, LD50, orl, frog (Sax 1986).	
Effects on invertebrates	LC50, 2 d:	
	0.492 mg/l	Ophiogomphus sp.
	0.099 mg/l	Pycnopsyche sp.
	0.124 mg/l	Simulium venustum
		(Poirier & Surgeoner 1987).
Effects on wastewater treatment	Not amenable to biological treatment at a municipal sewage treatment plant (Sax 1986).	
LOEC values to algae, mg/l	1–10	Oscillatoria terebriformis
		rpd, schr, Synechoccus lividus
		Navicula pelliculosa
		Scenedesmus quadricauda
		(Snyder & Sheridan 1974)
LC50 values to crustaceans, mg/l	0.01	48hr, Daphnia pulex (Sanders & Cope 1966)
	0.04	96hr, Gammarus fasciatus (Sanders 1972)
	0.01	Daphnia pulex (Kenaga 1979)
	0.076	48hr, scud (Sax 1986)
	1.2	96hr, Procambarus, 12 °C (Johnson & Finley 1980)
EC50 values to crustaceans, mg/l	0.0068	24hr, shrimp, 28 °C (Sax 1986)
	0.013	48hr, Simocephalus, 15 °C
	0.01	48hr, Daphnia pulex, 15 °C
	0.10–0.32	48hr, hard water, Daphnia pulex
		(Johnson & Finley 1980)

LC50 values to fishes, mg/l	8.1	96hr, Salmo trutta
	2.48	96hr, Perca fluviatilis
	10.2	96hr, Salmo gairdneri
	1.73	96hr, Oncorhyncus kisutch (Macek & McAllister 1970)
	16.2	96hr, Perca flavescens
	20	96hr, Salmo trutta m. lacustris (Mauck et al. 1977)
	15	act, Salmo gairdneri (Kenaga 1979)
	8.1	96hr, Salmo gairdneri
	1.7	96hr, Oncorhynchus kisutch
	2.9	96hr, Perca flavescens (Kemp et al. 1973)
	11.4	96hr, Ictalurus punctatus
	13.4	96hr, Cyprinus carpio
	14.7	96hr, Micropterus salmoides
	17	96hr, Pimephales promelas (Sax 1986)
	23	96hr, Oncorhynchus kisutch, 12 °C
	15.8	96hr, Salmo clarki, 10 °C
	12	96hr, Salmo gairdneri, 11 °C
	22.3	96hr, Salmo salar, 12 °C
	8.2	96hr, Salvelinus namaycush, 12 °C
	16.7	96hr, Lepomis cyanellus, 18 °C
	22.9	96hr, Lepomis macrochirus, 12 °C
	16.2	96hr, Perca flavescens, 12 °C
	7.2	96hr, Lepomis macrochirus, 12 °C
	0.32	96hr, Lepomis macrochirus, 12 °C (Johnson & Finley 1980)
Other information about water organisms	LC50 (96hr), 1.7 mg/l, Lymnea acuminata (Singh & Agarwal 1983). EC50 (96hr), 1.0 mg/l, oysters, shell growth (Sax 1986). LC50 (96hr), 0.010 mg/l, Pteronarcys, 15 °C (Johnson & Finley 1980). Delayed effect in recovery water, LC50, 0.04 d: Acroneuria sp., 0.251 mg/l; Isonychia sp., 0.356 mg/l; Ophiogomphus sp., 1.050 mg/l; Orconectes sp., 1.504 mg/l; Pycnopsyche sp., 0.430 mg/l; Simulium sp., 0.719 mg/l (Poirier & Surgeoner 1988).	

880 • 4-Dimethylamino-3,5-xylenol 6120-10-1

LC50 values to fishes, mg/l	7.2	96hr, Poecilia reticulata (Dave & Lidman 1978)

881 • 4-(1-(4-Dimethylamino-phenyl)-1-(4-methylaminophenyl)-methylene)-2,5-cyclohexadien-1-ylidene)-dimethylammonium-p-dodecyldiphenyl ether disulfonate

63428-00-2

Water solubility, mg/l	190 (MITI 1992)
Melting point, °C	162–181 (MITI 1992)
Log octanol/water coefficient, log Pow	2.6–3.1 (MITI 1992)
Total degradation in water	Biodegradation: 0–3% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	3.8–8.4 6w, Cyprinus carpio, conc 0.025 mg/l < 13–19 6w, Cyprinus carpio, conc 0.0025 mg/l (MITI 1992)
LC50 values to fishes, mg/l	0.872 48hr, Oryzias latipes (MITI 1992)

882 • Dimethylaminopyridine

1122-58-3

Synonyms	4-Dimethylaminopyridine
LD50 values to birds in oral exposure, mg/kg	> 100 orl-Agelaius phoeniceus (Schafer et al. 1983)
Other information about water organisms	EC50 (60hr), 530 mg/l, rpd, Tetrahymena pyriformis (Schultz & Mouton 1985).

883 • 2,4-Dimethylaniline

95-68-1

Sumformula of the chemical	C8H11N
pKa	4.87 (Sangster 1989)
Log octanol/water coefficient, log Pow	1.68 (Sangster 1989)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 8 mg/l (Bringmann & Kühn 1980a)
LOEC values to algae, mg/l	5 rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
Other information about water organisms	LOEC 9.8 mg/l, rpd, schr, Entosiphon sulcatum (Bringmann & Kühn 1980a). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 5 mg/l protozoa (Entosiphon sulcatum): 9.8 mg/l (Bringmann & Kühn 1980a)

884 • 2,5-Dimethylaniline 95-78-3

Sumformula of the chemical	C8H11N
EINECS-number	2024510
Water solubility, mg/l	5600 (MITI 1992)
Melting point, °C	12–13 (MITI 1992)
Boiling point, °C	213.5 (MITI 1992)
Log octanol/water coefficient, log Pow	1.91 (MITI 1992)
Total degradation in water	Biodegradation: 0–1% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	1.5–3.2 6w, Cyprinus carpio, conc 1 mg/l < 3.8 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
LC50 values to fishes, mg/l	239 48hr, Oryzias latipes (MITI 1992)

885 • 3,4-Dimethylaniline 95-64-7

Synonyms	3,4-Xylidine
Melting point, °C	48.9 (MITI 1992)
Total degradation in water	Biodegradation: 7.1% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).
Bioconcentration factor, fishes	1.9–3.3 6w, Cyprinus carpio, conc 1 mg/l < 10 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to birds in oral exposure, mg/kg	5.62 orl-Agelaius phoeniceus 10 orl-Sturnus vulgaris (Schafer et al. 1983)
LC50 values to fishes, mg/l	121 48hr, Oryzias latipes (MITI 1992)

886 • N, N-Dimethylaniline 121-69-7

Synonyms	Dimethylaniline (Dimethylamino)benzene N, N-Dimethylbenzeneamine Dimethylphenylamine Xylidene
Sumformula of the chemical	C8H11N

Use	Dyes, intermediates, solvent, manufacture of vanillin, stabilizer (acid acceptor), reagent.	
State and appearance	Yellowish to brownish, oily liquid.	
Molecular weight	121	
Specific gravity (water=1)	0.954	
Vapour density (air=1)	4.17	
Conversion factor, 1 ppm in air=	5.04	mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.2	ppm
Vapour pressure, mmHg	1 0.5	29.5 °C 20 °C
Water solubility, mg/l	1400	(MITI 1992)
Melting point, °C	2.5 > 1.9	 (MITI 1992)
Boiling point, °C	192.5	(MITI 1992)
Flashing point, °C	62.7	(closed cup)
pKa	5.15 5.1	25 °C (Sangster 1989)
Log octanol/water coefficient, log Pow	2.3 2.5 2.62 2.31	(Anon. 1986) (Anon. 1988) measured (Sax 1986) (Sangster 1989)
Henry's law constant, Pa x m^3/mol	6.8	(Anon. 1988)
Mobility	Equilibrium distribution: air water solid	 *mass %* 69.02 29.55 1.43 (Anon. 1988).
Other physicochemical properties	Soluble in alcohol and ether; insoluble in water; autoign temperature 370 °C. Combustible. Moderate fire hazard when exposed to heat, flame, or oxidation. When heated to decomposition it emits highly toxic fumes of aniline; it can react with oxidizing materials.	
Photochemical degradation in water	Flash photolysis of air-saturated aqueous solutions of N, N-dimethylaniline was examined at different pH values. Based on visual assessment, highly coloured permanent products were observed at pH values ranging between 2.6 and 6.3. No coloured products were observed at pH 1.6. With nitrogen-saturated solutions, the formation of these highly coloured products was not observed (Sax 1986).	
Oxidation-reduction reactions	The reactivity of N, N-dimethylaniline, as well as other compounds, with OH radicals in aqueous solution was compiled. The specific rate constant was reported as 5.3E+09/M sec. The temperature between 15–25 °C, pH was 9.0, and the method of detection was PNDA (Sax 1986).	
Half-life in water, days	2.3	in Rhine river water (Sax 1986)

Total degradation in water	Biodegradation: 1.9% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Other information about degradation	Biodegradation of N, N-dimethylaniline by activated sludge samples has been examined. Activated sludge samples were chosen from two treatment facilities that accepted domestic and industrial discharges. Sludges (3 ml) were dosed with 3 ml of N, N-DMA (final concentration of N, N-DMA = 20 mg/l) and incubated for 6hr at 25 °C. The concentration of N, N-DMA after incubation was determined by GLC or colorimetry. To distinguish bacterial degradation from other types, some of the sludge samples were sterilized by autoclave prior to incubation. Results: The average depletion of N, N-DMA from activated sludge samples was 1% and the depletion range was 0 to 3% (Sax 1986).
Bioconcentration factor, fishes	5.4–13.6 6w, Cyprinus carpio, conc 0.5 mg/l 4.7–10.1 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	990 orl-rat 1410 orl-rat (Sax 1986)
LD50 values to mammals in non-oral exposure, mg/kg	1700 dermal-rbt (Sax 1986)
LDLo values to mammals in oral exposure, mg/kg	50 orl-hmn (Sax 1986)
Health effects	Readily absorbed through skin and lungs (Sax 1986). Skin and eye irritation data: skn, rbt, 10 mg, 24hr, open, mild (Sax 1986).
LC50 values to fishes, mg/l	65.6 96hr, Pimephales promelas (Broderius & Kahl 1985) 102 48hr, Oryzias latipes (MITI 1992)
Other information about water organisms	EC50 110 mg/l, 24hr, rpd, Tetrahymena pyriformis (Yoshioka et al. 1985).

887 • 9,10-Dimethylanthracene 781-43-1

Sumformula of the chemical	C16H14
Log octanol/water coefficient, log Pow	5.69 (Sangster 1989)

888 • 7,12-Dimethylbenzanthracene 57-97-6

Synonyms	9,10-Dimethyl-1,2-benzanthracene
Sumformula of the chemical	C20H16
Log octanol/water coefficient, log Pow	5.8 (Sangster 1989)
Log soil sorption coefficient, log Kom	5.37 observed (Sabljic 1987) 5.83 calculated (Sabljic 1987)

LD50 values to birds in oral exposure, mg/kg	> 100 orl-Agelaius phoeniceus > 316 orl-Coturnix coturnix (Schafer et al. 1983)

889 • 3,3'-Dimethylbenzidine 119-93-7

Synonyms	Bianisidine
Sumformula of the chemical	C14H16N2
Molecular weight	212.32
Water solubility, mg/l	50 (MITI 1992)
Melting point, °C	129 (MITI 1992)
Log octanol/water coefficient, log Pow	2.39 (MITI 1992)
Total degradation in water	Biodegradation: 3% by BOD substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	4.8–34 8w, Cyprinus carpio, conc 0.2 mg/l 10–83 8w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	404 orl-rat (Lewis & Sweet 1984)
LDLo values to mammals in oral exposure, mg/kg	600 orl-dog (Lewis & Sweet 1984)
LDLo values to mammals in non-oral exposure, mg/kg	125 ipr-rat (Lewis & Sweet 1984) 125 ipr-mus (Lewis & Sweet 1984)
TDLo values to mammals in oral exposure, mg/kg	4500 orl-rat (Lewis & Sweet 1984)
TDLo values to mammals in non-oral exposure, mg/kg	3240 scu-rat (Lewis & Sweet 1984) 5040 imp-rat (Lewis & Sweet 1984)
Carcinogenicity	Carcinogenic determination: animal positive (Lewis & Sweet 1984).
LC50 values to fishes, mg/l	56 48hr, Oryzias latipes (MITI 1992)

890 • N, N-Dimethylbenzylamine 103-83-3

Sumformula of the chemical	C9H13N
EINECS-number	2031491
Water solubility, mg/l	12000 (MITI 1992)
Melting point, °C	< -10 (MITI 1992)
Boiling point, °C	181 (MITI 1992)
Log octanol/water coefficient, log Pow	1.54–1.91 (MITI 1992)

Total degradation in water	Biodegradation: 0–2% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	2.1–6.4 6w, Cyprinus carpio, conc 0.5 mg/l < 6.2–22 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
LC50 values to fishes, mg/l	59.3 48hr, Oryzias latipes (MITI 1992)

891 • Dimethylformamide 68-12-2

Synonyms	DMF DMFA N, N-Dimethylmethanamide
Sumformula of the chemical	C3H7NO
Use	Solvent.
Boiling point, °C	153 (MITI 1992)
Log octanol/water coefficient, log Pow	-1.01 (Sangster 1989)
Volatilization	Relative volatility (nBuAc=1) = 0.2
Total degradation in water	Biodegradation: 4.4% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Bioconcentration factor, fishes	0.3–0.8 8w, Cyprinus carpio, conc 0.02 mg/l 0.3–1.2 8w, Cyprinus carpio, conc 0.002 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	2800 orl-rat
LC50 values to crustaceans, mg/l	13000 48hr, Daphnia magna (LeBlanc & Surprenanat 1983)
LC50 values to fishes, mg/l	9800 48hr, Oryzias latipes (MITI 1992)

892 • 2,5-Dimethylhexa-2,4-diene 764-13-6

Sumformula of the chemical	C8H14
Water solubility, mg/l	32 (MITI 1992)
Log octanol/water coefficient, log Pow	3.5 (MITI 1992)

Total degradation in water	Biodegradation (Closed Bottle Test): 4% by BOD period: 28d substance: 1.6 mg/l sludge: 2 mg (AS)/l 3% by BOD period: 28d substance: 7.7 mg/l sludge: 2 mg (AS)/l (MITI 1992).
Bioconcentration factor, fishes	155–493 8w, Cyprinus carpio, conc 0.04 mg/l 150–266 8w, Cyprinus carpio, conc 0.004 mg/l (MITI 1992)
LC50 values to fishes, mg/l	4.3 48hr, Oryzias latipes (MITI 1992)

893 • 1,1-Dimethylhydrazine

57-14-7

Synonyms	Dimazine n, n-Dimethylhydrazine UDMH
Sumformula of the chemical	C2H8N2
Use	Major use as a storable, high-energy propellant for liquid-fuelled rockets. Apollo rocket fuel was 50:50 mixture of UDMH and hydrazine with nitrogen tetroxide as the oxidizer. Also used in the manufacture of N-dimethylaminosuccinamic acid, a plant growth regulator to retard growth of ornamentals such as chrysanthemums and to control the vegetation, flowers, or fruits of food crops, e.g. apples, grapes, peanuts, cherries, peaches, and tomatoes. Also may be used to manufacture aminimides. Photographic chemicals, as a stabilizer for fuel additives, and as an absorbent for acid gases.
State and appearance	Hygroscopic mobile liquid. Fuming, colourless liquid. Clear. Gradually turns yellow. Floats and mixes with water.
Odour	Fishy or amine-like odour. Odour threshold, lower: 6 ppm; Odour threshold, upper: 14 ppm (Sax 1986). 100% odour recognition level: 41300 ppm at 20 °C (Sax 1986).
Specific gravity (water=1)	0.791 0.782
Vapour density (air=1)	2.1
Vapour pressure, mmHg	103 157 25 °C 10 -22 °C
Melting point, °C	-57
Boiling point, °C	63.9 62.5
Log octanol/water coefficient, log Pow	-1.9 (Sax 1986)

Adsorption/desorption	UDMH is strongly absorbed and/or decomposed on clay particles. The decomposition of UDMH is accelerated by soils as well as by Montmorillonite and kaolinite clays. In dilute solutions, UDMH can be absorbed and/or decomposed in a relatively short column of soil containing a moderate amount of clay. Slowly permeable clay soils are likely to prevent spills of UDMH from reaching groundwater and to minimize runoff. However, in large-scale runoff of rainfall waters, absorbed UDMH may be carried off in the colloidal clay fraction (Sax 1986). Flammability: Quite flammable. Easily ignited. The mixture with hydrazine may catch fire spontaneously if spilled. Flammable in air. Ignites spontaneously in contact with oxidizing agents. Flashback along vapour trail may occur. Burning rate is 3.8 mm/minute (Sax 1986). Toxic combustion products: Poisonous gases (toxic nitrogen oxides) are produced when heated and during combustion. Incomplete oxidation may give hazardous decomposition products (hydrogen, ammonia, dimethylamine, hydroazoic acid (Sax 1986). Explosiveness: Reaction with oxidizers is explosive. Vapour may explode if ignited in an enclosed area. Prolonged exposure of containers of UDMH to fire or heat may result in their violent rupturing and rocketing due to its decomposition. Shock insensitive (Sax 1986). Misciple with water with evolution of heat (Sax 1986).
Other chemical degradation processes	1,1-dimethylhydrazine reacts slowly with molecular oxygen in the presence of ultraviolet irradiation. Oxidation by molecular oxygen in water will convert hydrazines to diimines and, ultimately, to nitrogen gas. The reaction is catalyzed by metal ions, particularly copper. As a result, 1,1-dimethylhydrazine is not expected to be an environmentally persistent substance. – Hydrazines do not photolyze in the solar actinic region (wavelength > 290 nm). Reactions with OH radical and ozone are their likely pathways in the atmosphere. The latter is the major fate. The major product (60% yield within 2 to 3 minutes) in the reaction of ozone with UDMH under simulated atmosperic conditions is dimethylnitrosamine, which upon irradiation gives dimethylnitramine (CH3)2NNO2: Formaldehyde, nitrogen oxides, and nitrous acid. Other products from the reaction of ozone with UDMH are formaldehyde and hydrogen peroxide. Similar products are formed during photooxidation of UDMH in the presence of NO. Another possible product in N-nitrosodimethylhydrazine (Sax 1986). Water solutions are weakly alkaline. – UDMH forms salts with mineral acids. It is a strong reducing agent oxidized by compounds such as peroxides, iodates, ferricyanide, and ceric ions in acid solution. – UDMH was oxidized in distilled water and sterilized and unsterilized lake water. Oxidation in distilled water occurred in the presence or absence of the cupric ion. Oxidation products in lake water were further degraded when microorganisms were present. - Ozonation of UDMH gives methanol, formaldehyde dimethylhydrazone, formaldehyde monomethylhydrazone, N-nitrosodimethylamine, dimethyl formamide, and tetramethyl tetrazene. Ozonation reduces the toxicity to fish and daphnia (Sax 1986).
Other information about bioaccumulation	Based on a low octanol/water partition coefficient 1,1-dimethylhydrazine should not bioaccumulate. However 1,1-dimethylhydrazine is rapidly absorbed into the blood of dogs and declines very slowly after reaching a peak value which possibly indicates binding to cellular constituents and deposition in adipose tissue (Sax 1986).
LD50 values to mammals in non-oral exposure, mg/kg	102 ipr-rat 125 ipr-mus 12 scu-mus (Sax 1986)
LC50 values to mammals in inhalation exposure, ppm	252 ihl-rat, 4hr 172 ihl-mus, 4hr 3580 ihl-dag, 15min 392 ihl-ham, 4hr (Sax 1986)

LDLo values to mammals in non-oral exposure, mg/kg	30 ipr-cat (Sax 1986)
TDLo values to mammals in oral exposure, mg/kg	150 orl-rat, 7W-I, tumorigenic 5880 orl-mus, 42W-C, tumorigenic 228000 orl-ham, 48W-C, tumorigenic (Sax 1986)
TDLo values to mammals in non-oral exposure, mg/kg	21 scu-rat, tumorigenic 144 ipr-mus, 8W-I, tumorigenic (Sax 1986)
Health effects	Target organs are the central nervous system, gastrointestinal tract, blood, respiratory system, eyes, and skin (Sax 1986). Vapour irritates eyes, skin, and respiratory tract. – Contact with eyes, skin, or mucous membranes causes chemical burns. Severe skin irritant effect causes second- and third-degree burns on short contact. Very injurious to the eyes. Can be absorbed through skin to cause systemic intoxication and convulsions (Sax 1986). Breathing of vapour causes pulmonary irritation, delayed gastrointestinal irritation, tremors, and conculsions. Moderately irritating on inhalation. Personnel will not usually tolerate moderate or high air concentrations. – Choking, chest pain, difficulty in breathing, lethargy, nausea, anoxia, liver injury. – Minimum exposure symptoms: upper respiratory irritation and muscle tremors. Acute symptoms, excitement, tremors and conculsions. – Respiratory irritation leads to pulmonary edema in some human cases. Headache and vomiting may occur. Liver toxicity indicated by a positive cephalin flocculation test, raised serum glutamic pyruvic transaminase (SGPT), fatty degeneration in liver biopsies. The liver toxicity is believed to be due to the formation of dimethylnitrosamine. The only continuing effects of acute human toxicity besides liver injury were complaints of persistent UDMH odour and taste in the mouth (Sax 1986).
Carcinogenicity	Carcinogenic in mice after oral dosing. A proper evaluation of carcinogenicity in rats could not be made because the doses were high and only a few liver tumors occurred after a long latent period. No epidemiological information was available to assess human carcinogenicity. – After a lifetime study, most mice had tumors of the blood vessels (more than half in the liver; most were angiosarcomas) or lungs (Adenomas and a few adenocarcinomas) and some had kidney and liver tumors (Sax 1986).
Mutagenicity	Not mutagenic in the dominant lethal mutation test in mice. Did not produce abnormalities in sperm of mice. A UDMH metabolite was mutagenic to microorganisms in a battery tests (Sax 1986). Mutagen data: mmo, sat, 0.042 mmol/plate; mma, sat, 0.042 mmol/plate; mmo, esc, 0.020 mmol/l; dnr, esc, 0.020 ml/disc; dnd, esc, 0.001 mmol/l; pic, esc, 17000 mg/l; dnr, bcs, 0.020 ml/disc; mmo, asn, 250 nl/plate; dns, rat, ipr, 60 mg/kg; dnd, mus, ipr, 3.5 mmol/kg; dni, mus, orl, 200 mg/kg; msc, mus, lym, 5 mmol/l, 24hr; hma, mus, sat, 125 mg/kg (Sax 1986).
Teratogenicity	No mammalian teratogenicity data were found in a 1980 literature survey. UDMH was teratogenic to South Africal clawed toad (Xenopus laevis) embryos (Sax 1986).

Effects on plants	Cotton seedlings grown in water containing 1000 ppm UDMH showed a general flaccidity of the leaves, dehydration, and death at 48 hours. True leaves and cotyledons became necrotic. When applied as a spray to the drip point on endive, soybean, pinto bean, squash, and cotton plants, gave injury indexes (on a scale of 0 for no injury to 8 for death) of 0 to 2 after 5 days of 2000 ppm, 0 to 4 after 5 days at 6000 ppm, and 0 to 4 after 5 days at 10000 ppm. Injury, when it occurred, developed within the first day as scattered necrotic spotting and, occasionally, leaf curl (Sax 1986). Seedlings of cotton, pinto bean, soybean, and squash suffer severe injury upon exposure to 25 to 30 ppm UDMH (Sax 1986).
Effects on wastewater treatment	Biological waste treatment detoxification of UDMH is not recommended. Spills could be expected to disrupt the natural bacterial balance in the aquatic environment and probably sewage treatment systems (Sax 1986).
EC50 values to crustaceans, mg/l	5 5-10, 48hr, Daphnia magna 10 first instar, pH 8.1 (Sax 1986)
LC50 values to fishes, mg/l	10.1 hrd, act, 96hr, Poecilia reticulata 26.5 sfd, act, 96hr, Poecilia reticulata (Slonium 1977) 0.35 96hr, Pimephales promelas (Sax 1986)
Other information about water organisms	100 ppm UDMH caused a marked growth decrease in cultures of the alga Chlorella pyrenoidosa (Sax 1986).
Other information	Flammable, explosive, toxic, a carcinogen, a mutagen, and a teratogen (Sax 1986).

894 • Dimethylnitrooxopropyran carboxylic acid ester 6272-87-3

Other information about mammals	ALD = 100.0 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987).

895 • N, N-Dimethylnitrosoamine 62-75-9

Carcinogenicity	Carcinogenic (Anon. 1974, McCann et al. 1975)
Other information about water organisms	LD50 1770 mg/kg, Salmo gairdneri (Grieco et al. 1978).

896 • Dimethylphosphate 813-78-5

LC50 values to fishes, mg/l	18	96hr, Pimephales promelas (Kemp et al. 1973)

897 • Dimethylphosphite 868-85-9

LC50 values to fishes, mg/l	225	96hr, Pimephales promelas (Kemp et al. 1973)

898 • Dimethylphthalate 131-11-3

Use	Solvent and various.	
Molecular weight	194	
Water solubility, mg/l	1800	(MITI 1992)

Melting point, °C	-0.1 (MITI 1992)
Boiling point, °C	283.5–284.0 (MITI 1992)
Log octanol/water coefficient, log Pow	1.5 (Anon. 1988)
Henry's law constant, Pa x m³/mol	0.011 (Anon. 1988)
Mobility	Equilibrium distribution: *mass %* air 0.37 water 99.15 solid 0.48 (Anon. 1988).
Total degradation in water	Biodegradation: 90–98% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
LD50 values to birds in oral exposure, mg/kg	> 100 orl-Agelaius phoeniceus (Schafer et al. 1983)
LC50 values to crustaceans, mg/l	62 96hr, Nitocra spinipes (Linden et al. 1979) 33 48hr, Daphnia magna (LeBlanc 1980) 100 8d, Palaemonetes pugio (Laughlin et al. 1978)
LC50 values to fishes, mg/l	50 96hr, Lepomis macrochirus (Buccafusco et al. 1981) 100–115 96hr, Alburnus alburnus (Linden et al. 1979) 58 96hr, Cyprinodon variegatus (Heitmuller et al. 1981)

899 • S,S'-2-Dimethylpropane-1,3-diyl dithiocarbamate 15263-53-3

Sumformula of the chemical	C7H15O2N3S2
Water solubility, mg/l	> 2.5 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD, disulfidized to 4-(N, N-Dimethylamino)-1,2-dithiolane period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

900 • 4,6-Dinitro-o-cresol 534-52-1

Synonyms	4,6-Dinitro-2-cresol 2,4-Dinitro-6-methylphenol 2-Methyl-4,6-dinitrophenol 2,4-Dinitro-o-cresol 3,5-Dinitro-2-hydroxytoluene Dinitromethylcyclohexytrienol o-Dinitrocresol
Sumformula of the chemical	C7H6N2O5

Use	On dormant plants or on waste ground as an ovicide, insecticide, and as a broad leaf herbicide. It is used as a defoliant on actively growing plants and as a blossom thinner and a preventer of alternate bearing fruit trees. It is also used as a fungicide, acaricide, and in scab apple control.
State and appearance	Yellow prisms. In water: colourless aqueous solution turns yellow when alkaline.
Molecular weight	198.15
Vapour density (air=1)	6.8
Vapour pressure, mmHg	0.000052
Water solubility, mg/l	200 (MITI 1992)
Melting point, °C	84–86 (MITI 1992)
Log octanol/water coefficient, log Pow	2.85 (Sax 1986) 1.86 (MITI 1992)
Other physico–chemical properties	Dinitrophenols are stable at low pH, but decompose upon ultraviolet radiation in alkaline solutions. – DNOC rapidly forms water soluble ammonium, sodium, potassium, and calcium salts. – Although it is slow, photolysis is the main process of DNOC breakdown in an aqueous environment. Bacterial breakdown may be very slow in water. DNOC does absorb on clay and may hydrolyse during sorption (Sax 1986).
Other information about degradation	Biodegradation: adapted culture: 1% removal after 48hr incubation (feed 207 mg/l). Photolysis is thought to be the main route of degradation in an aquatic environment. No half-life is given but the process is described as slow. The time of disappearance in soil is from a few weeks to 2 months (Sax 1986).
Metabolism in mammals	The half-life in man is 5.78 days (Sax 1986).
Other information about metabolism	Most organisms reduce a NO2 grout to NH2. This process is most significant in microorganisms and fish (Sax 1986).
Bioconcentration factor, fishes	< 0.3–0.7 6w, Cyprinus carpio, conc 0.05 mg/l < 2.9 6w, Cyprinus carpio, conc 0.005 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	10 orl-rat 47 orl-mus (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	200 skn-rat 19 ipr-mus (Lewis & Sweet 1984)
LDLo values to mammals in non-oral exposure, mg/kg	29 unk-man 28 ipr-rat 15 ivn-dog (Lewis & Sweet 1984) 500 skn-gpg (Sax 1986)
LCLo values to mammals in inhalation exposure, mg/kg	40 ihl-cat (Lewis & Sweet 1984)
TCLo values to mammals in inhalation exposure, mg/kg	1 ihl-hmn (Lewis & Sweet 1984)
Effects on the physiology of mammals	DNOC uncouples the oxidation of cytochrome B by flavoprotein during oxidative phosphorylation in both animals and plants. 1 mg/m³ has resulted in central nervous system effects in humans. DNOC produces hyperpyrexia, hyperglycemia, glycouria, kidney damage, cardiovascular changes and gastrointestinal tract changes (Sax 1986).

Health effects	Symptoms of poisoning include deep, rapid respiration, sweating, thirst, heat sensation, motor weakness, collapse, coma, and death. Rigor mortis occurs early. The poison action is cumulative. Chronic poisoning symptoms include cataracts, chest pain, dermatitis, dyspnea, fever, jaundice, nausea and vomiting, flushing, weight loss, headache, diarrhea, kidney damage, cardiovascular changes, gastrointestinal tract changes, central nervous system effects, hyperpyrexia, hyperglycemia, and glycosuria (Sax 1986). Skin and eye irritation data: skn, rbt, 105 mg, 9 D-I, mild; eye, rbt, 20 mg, 24hr, severe (Sax 1986).
Mutagenicity	Salmonella, T4 bacteriophage and two R III mutagens of the T4 bacteriophage did not produce mutations when treated with dinitro-o-cresol. Escherichia coli did not produce mutagens but there is evidence of DNA damage to proteus (Sax 1986). Mutagen data: mmo, sat, 0.050 ml/plate; snr, omi, 10 mg/plate; sln, dmg, orl, 0.250 mmol/l (Sax 1986).
Other information about birds	lvn-pgn, LDLO 7 mg/kg (Sax 1986).
Effects on amphibia	NOEC, 0.32 mg/l, 100d, Xenopus laevis, mortality. NOEC, 0.32 mg/l, 100d, Xenopus laevis, development. NOEC, 0.32 mg/l, 100d, Xenopus laevis, growth. (Slooff & Canton 1983)
Effects on arthropods	NOEC, 10 mg/l, 25d, Culex pipiens, mortality. NOEC, 10 mg/l, 25d, Culex pipiens, development. (Slooff & Canton 1983)
Effects on plants	Irrigable plants: as an herbicide, DNOC primarily produces local root damage. The first effect in solution is to reduce transpiration drastically. Dinitrophenols inhibit oxidative phosphorylation. DNOC inhibits pollen tube growth, prevents pollen generation, and injures the stigma so that it cannot function (Sax 1986). NOEC, 0.32 mg/l, 7d, Lemna minor, specific growth rate. (Slooff & Canton 1983)
Effects on microorganisms	NOEC, 10 mg/l, 0.3d, Pseudomonas fluorescens, specific growth rate. NOEC, 3.2 mg/l, 4d, Microcystis aeruginosa, specific growth rate. (Slooff & Canton 1983) Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 16 mg/l (Bringmann & Kühn 1980a)
Other effects on terristrial ecosystems	Adsorption of DNOC by clays is pH dependent. At pH 4.6 the adsorption is > 99% on illite and montmorillonite clays. No adsorption at pH 7.3. Cultures of Arthrobacter simplex and Pseudomonas sp. metabolize DNOC. A pseudomonad reduced DNOC by progressive reduction and deamination. A. simplex degraded DNOC by oxidative elimination of the two nitro groups. The two pathways converge until ring cleavage and the fission products were identical. Concentrations of 40–2000 ppm inhibit growth of soil actinomycetes, bacteria and fungi. Only 40 ppm inhibited Cytophaga sp. and Mucor sp.; > 400 ppm inhibits Bacterium subtilis, B. mycoides, and Actinomyces sp. Effects on numbers of soil fungi and bacteria is only transitory. At 25 ppm DNOC in soil inhibited nitrogen-fixing capacity for about 2 mos. – Soil treated with DNOC at 6 kg/ha showed increased numbers of collembola and soil mites after 9 months after initial toxicity. Though all population eventually increased, folsoma were most susceptible to DNOC. Tullsergia were less susceptible but hypogastrua thrived. The increase in population is attributed to an increase on the bacteria, fungi, and nematode population which is a food source for mites and springtails. DNOC is harmless to carbid predators. – DNOC is toxic to Lumbricus castaneus but harmless to Allolobophora caliginosa (both earthworms). – The time for disapperance in soil is a few weeks to two months. – Degradation takes place more quickly in soils previously treated with DNOC than in other soils. Soil with a previous DNOC treatment loses 90% in 11 days. Soils without a previous DNOC treatment loses 90% in 15 days (Sax 1986).

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LOEC values to algae, mg/l	0.15	rpd, schr, Microcystis aeruginosa (Bringmann & Kuhn 1976)
NOEC values to algae, mg/l	3.2	grw, schr, 96hr, Microcystis aeruginosa (Slooff & Canton 1983)
	10	4d, grw (biomass), Scenedesmus pannonicus (Slooff & Canton 1983)
LC50 values to crustaceans, mg/l	3.1	48hr, Daphnia magna (LeBlanc 1980)
	3.3	48hr, Daphnia magna (Hermens et al. 1984)
	4.3 3.1 3.12 1.1	24hr, Daphnia magna CaC03, 173 mg/l 48hr, Daphnia magna CaC03, 173 mg/l 48hr, Daphnia (Sax 1986)
		96hr, Gammarus fasciatus, 21 °C (Johnson & Finley 1980)
EC50 values to crustaceans, mg/l	2.1	rpd, schr, 16 d, Daphnia magna (Hermens et al. 1984)
	0.145	48hr, Daphnia pulex, first instar, 21 °C (Johnson & Finley 1980)
NOEC values to crustaceans, mg/l	1	srv, chr, 21 d, Daphnia magna (Slooff & Canton 1983)
	1	rpd, 21d, Daphnia magna (Slooff & Canton 1983)
LC50 values to fishes, mg/l	0.23	96hr, Lepomis macrochirus (Buccafusco et al. 1981)
	8.6 1.9–2.2	48hr, Pimephales promelas 96hr, Pimephales promelas (Phipps et al. 1981)
	0.23 2.04 0.23 0.21	96hr, Lepomis macrochirus 96hr, Pimephales promelas 96hr, Lepomis macrochirus 48hr, Salmo gairdneri (Sax 1986)
	0.066 0.36	96hr, Salmo gairdneri, 13 °C 96hr, Lepomis macrochirus (Johnson & Finley 1986)
	1.8	48hr, Oryzias latipes (MITI 1992)
LOEC values to fishes, mg/l	0.2	srv, act, Salmo salar (Zitko et al. 1976)
NOEC values to fishes, mg/l	1 1 1 0.1 0.1 1	28d, srv, Poecilia reticulata 28d, srv + bhv, Poecilia reticulata 28d, grw, POecilia reticulata 40d srv, Oryzias latipes 40d, srv + bhv, Oryzias latipes 40d, grv, Oryzias latipes (Slooff & Canton 1983)
Other information about water organisms	LC50 0.00032 mg/l, 96hr, Pteronarcys californica; LD50 4.2 mg/l, 48hr, Cloeon, dipterum nymph (Sax 1986). NOEC, 0.32 mg/l, 21d, Hydra oligactis, specific growth rate. NOEC, 1 mg/l, 40d, Lymnaea stagnalis, mortality. NOEC, 0.032 mg/l, 40d, Lymnaea stagnalis, reproduction. NOEC, 1 mg/l, 40d, Lymnaea stagnalis, hatching. (Slooff & Canton 1983) Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 13 mg/l protozoa (Entosiphon sulcatum): 5.4 mg/l (Bringmann & Kühn 1980a)	

Other effects on aquatic ecosystems	0.001 ppm the proposed 1976 EPA water quality criteria set the allowable level of DNOC at 0.001 mg/l to protect against fish tainting (Sax 1986).	

901 • 4,6-Dinitro-o-sec-amylphenol 4097-36-3

Synonyms	DNAP	
Use	Herbicide.	
LOEC values to fishes, mg/l	30	srv, act, Salmo salar (Zitko et al. 1976)

902 • 3,5-Dinitroaniline 618-87-1

Molecular weight	183.14	
LOEC values to algae, mg/l	0.13	rpd, 5 d, Selenastrum capricornutum (van der Shalie 1983)
EC50 values to crustaceans, mg/l	3.8 14.7	rpd, 48hr, Daphnia magna (van der Shalie 1983) mbt, 48hr, Daphnia magna (Pearson et al. 1979)
LC50 values to fishes, mg/l	3 21.4	96hr, Salmo gairdneri (van der Shalie 1983) 96hr, Pimephales promelas (Pearson et al. 1979)
LOEC values to fishes, mg/l	0.65	phy, 71 d, Salmo gairdneri, van der Shalie

903 • Dinitrobenzene 25154-54-5

Sumformula of the chemical	C6H4O4N2	
EINECS-number	2466736	
Melting point, °C	118	(MITI 1992)
Boiling point, °C	319	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).	
Bioconcentration factor, fishes	< 2.2–4.9 < 22–37.4	6w, Cyprinus carpio, conc 0.05 mg/l 6w, Cyprinus carpio, conc 0.005 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-acculuative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	3.3	48hr, Oryzias latipes (MITI 1992)

904 • 1,2-Dinitrobenzene 528-29-0

Other information about water organisms	EC50 (60hr), 9.4 mg/l, rpd, Tetrahymena pyriformis (Schultz & Applehans 1985).	

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905 • 1,3-Dinitrobenzene 99-65-0

Synonyms	m-Dinitrobenzene m-Nitrobenzene	
State and appearance	Colourless yellowish needles.	
Molecular weight	168.12	
Water solubility, mg/l	469	15 °C
Melting point, °C	89.8	
Boiling point, °C	300–302	
Total degradation in soil	Biodegradation: decomposition by a soil microflora in > 64 days (Verschueren 1983).	
LD50 values to mammals in oral exposure, mg/kg	83	orl-rat (Lewis & Sweet 1984)
LDLo values to mammals in oral exposure, mg/kg	27 600	orl-cat orl-dog (Lewis & Sweet 1984)
TDLo values to mammals in non-oral exposure, mg/kg	4	2 d, skn-man (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	42 42.2 > 100	orl-bwd (Lewis & Sweet 1984) orl-Agelaius phoeniceus orl-Sturnus vulgaris (Schafer et al. 1983)
Maximum longterm immission concentration in air for plants, mg/m³	0.035	VDI 2306
Maximum longterm immission concentration in air for plants, ppm	0.005	VDI 2306
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 14 mg/l (Bringmann & Kühn 1980a).	
LOEC values to algae, mg/l	0.7 0.1 0.97	rpd, schr, Scenedesmus quadricauda rpd, schr, Microcystis aeruginosa (Bringmann & Kuhn 1976) rpd,5 d, Selenastrum capricornutum (van der Shalie 1983)
LC50 values to crustaceans, mg/l	27 43	48hr, Daphnia magna (van der Shalie 1983) 48hr, Daphnia magna (Hermens et al. 1984)
EC50 values to crustaceans, mg/l	3.2 53	srv,16 d, Daphnia magna (Hermens et al. 1984) mbt, 48hr, Daphnia magna (Pearson et al. 1979)
LC50 values to fishes, mg/l	1.7 12.7 7.4	96hr, Salmo gairdneri (van der Shalie 1983) act, Pimephales promelas (Curtis & Ward 1981) act, Pimephales promelas (Pearson et al. 1979)
LOEC values to fishes, mg/l	0.42	srv, 30 d, Salmo gairdneri (van der Shalie 1983)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 0.7 mg/l protozoa (Entosiphon sulcatum): 0.76 mg/l (Bringmann & Kühn 1980a).	

906 • 1,4-Dinitrobenzene 100-25-4

LC50 values to fishes, mg/l	0.6 96hr, Pimephales promelas 0.673 96hr, Ictalurus punctatus (Holcombe et al. 1984)
Other information about water organisms	EC50 (60hr), 7.3 mg/l, rpd, Tetrahymena pyriformis (Schultz & Applehans 1985) LC50, 4.24 mg/l, 96hr, snail (Holcombe et al. 1984)

907 • Dinitrobutylphenol 51053-28-2

LC50 values to crustaceans, mg/l	18 96hr, Gammarus fasciatus (Kemp et al. 1973)

908 • Dinitrophenol 25550-58-7

Molecular weight	184.12
LDLo values to mammals in oral exposure, mg/kg	30 orl-rat 30 orl-dog (Lewis & Sweet 1984)
LC50 values to crustaceans, mg/l	6.85 96hr, Saccobranchus fossilis (Verma et al. 1980a)
LC50 values to fishes, mg/l	1.34 96hr, Notopterus notopterus (Verma et al. 1981b) 8.6 96hr, Channa punctata (Verma et al. 1980a)
LOEC values to fishes, mg/l	0.7 srv, act, Salmo salar (Zitko et al. 1976)

909 • 2,4-Dinitrophenol 51-28-5

Synonyms	2,4-DNP
State and appearance	Yellow rhombic crystals or needles.
Molecular weight	184.12
Water solubility, mg/l	5600 18 °C 540 (MITI 1992)
Melting point, °C	111.5–115.5 (MITI 1992)
Log octanol/water coefficient, log Pow	1.5 Anon. 1986 1.05 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

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Other information about degradation	Biodegradation:adapted culture: 2% removal after 48hr incubation, feed: 200 mg/l (Verschueren 1983).

Degradation of 2,4-dinitrophenol (+ adapted to parathion):

ENVIRONMENT	*INIT.CONC. mg/l*	*REDOX-COND.*	*TEMP. °C*	*DEGRADATION %/day*	*REF.*
water	5	aerobic	25	60/7	a
water	10	aerobic	25	68/7	a
water (adapted)	5	aerobic	25	100/7	a
water (adapted)	10	aerobic	25	100/7	a
sludge	550	aerobic	-	appr. 80/100	b
sludge	1000	aerobic	-	appr. 50/75	b
sludge	4000	aerobic	-	70/125	b
soil	23	aerobic	28	74/10	c
soil (adapted+)	23	aerobic	28	100/10	c
soil	22	aerobic	28	100/10	c
soil (adapted+)	21	aerobic	28	100/5	c

a) Tabak et al. 1981 b) Kincannon & Lin 1985
c) Sudhakar-Barik et al. 1979 (Anon. 1987b).

Bioconcentration factor, fishes	< 0.4–0.7	6w, Cyprinus carpio, conc 0.05 mg/l
	< 3.7	6w, Cyprinus carpio, conc 0.005 mg/l (MITI 1992)
LD50 values to mammals in oral exposure, mg/kg	30	orl-rat
	45	orl-mus
	30	orl-rbt (Lewis & Sweet 1984)
LDLo values to mammals in oral exposure, mg/kg	30	orl-dog (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	13	orl-bwd (Lewis & Sweet 1984)
	13.3	orl-Agelaius phoeniceus
	42.2–46.0	orl-Sturnus vulgaris
	≥ 9.00	orl-Passer domesticus (Schafer et al. 1983)
Effects on arthropods	Tanytarsus dissimilis; 2 d, LC50, > 48.1 mg/l (Olsson & Haux 1986).	
Effects on plants	2,4-DNP was phytotoxic with germination effects appearing at 40 ppm (dry soil basis) for soybean. The fresh top weight of corn, soybean and fescue were decreased by 2,4-DNP at 20–40 ppm (dry soil basis) (Overcash et al. 1981).	
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 115 mg/l (Bringmann & Kühn 1980a)	
LOEC values to algae, mg/l	16	rpd, schr, Scenedesmus quadricauda (Bringmann & Kuhn 1980a)
LC50 values to crustaceans, mg/l	4.1	48hr, Daphnia magna (LeBlanc 1980)
	> 48.1	4d, Orconectes immunis (Holcombe et al. 1987)
EC50 values to crustaceans, mg/l	4.39	2d, mbt, Daphnia magna (Holcombe et al. 1987)

LC50 values to fishes, mg/l	0.62	96hr, Lepomis macrochirus (Buccafusco et al. 1981)
	29	96hr, Cyprinodon variegatus (Heitmuller et al. 1979)
	7.3	48hr, Pimephales promelas (Phipps et al. 1981)
	23	4d, Carassius auratus
	8.39	4d, Pimephales promelas
	3.97	4d, Lepomis macrochirus
	1.16	4d, Salmo gairdneri
	> 4.59	4d, Catostomus commersoni (Holcombe et al. 1987)
	2.07	2d, Salmo gairdneri (McKim et al. 1987)
	19.1	48hr, Oryzias latipes (MITI 1992)
LOEC values to fishes, mg/l	0.7	srv, act, Salmo salar (Zitko et al. 1976)
Other information about water organisms	Aplexa hypnorum; LC50, 4 d, 6.49 mg/l (Holcombe et al. 1987). Lethal threshold concentration (LT50): 0.63 d, 4.64 mg/l, Salmo gairdneri (McKim et al. 1987). Tetrahymena pyriformis; EC50, grw, 14.77 mg/l, 2d (Schultz 1987). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 16 mg/l protozoa (Entosiphon sulcatum): 20 mg/l (Bringmann & Kühn 1980a)	

910 • 2,5-Dinitrophenol 329-71-5

Other information about water organisms	Tetrahymena pyriformis; EC50, grw, 2 d, 21.68 mg/l (Schultz 1987).

911 • N, N'-Dinitrosopentamethylene tetramine 101-25-7

Sumformula of the chemical	C5H10N6O2
EINECS-number	2029283
Water solubility, mg/l	5700 (MITI 1992)
Melting point, °C	204–205 (MITI 1992)
Total degradation in water	Biodegradation: 63–66% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

912 • Dinitrotoluene 25321-14-6

Synonyms	Methyldinitrobenzene
Sumformula of the chemical	C7H6N2O4
EINECS-number	2468361
Melting point, °C	56–59 (MITI 1992)

Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Bioconcentration factor, fishes	0.6–2.9 8w, Cyprinus carpio, conc 0.25 mg/l 3.2–21.2 8w, Cyprinus carpio, conc 0.025 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	27 48hr, Oryzias latipes (MITI 1992)

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913 • 2,3-Dinitrotoluene 602-01-7

Molecular weight	182.15	
Melting point, °C	59–61	
LD50 values to mammals in oral exposure, mg/kg	911 1072	orl-rat orl-mus (Lewis & Sweet 1984)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 9 mg/l (Bringmann & Kühn 1980a)	
LOEC values to algae, mg/l	0.22 0.83	rpd, schr, Microcystis aeruginosa (Bringmann & Kuhn 1976) rpd, schr, Scenedesmus quadricauda (Bringmann & Kuhn 1980a)
LC50 values to crustaceans, mg/l	0.66	48hr, Daphnia magna (LeBlanc 1980)
EC50 values to crustaceans, mg/l	4.7	mbt, 48hr, Daphnia magna (Pearson et al. 1979)
LC50 values to fishes, mg/l	0.33 2.3 1.9	96hr, Lepomis macrochirus (Buccafusco et al. 1981) 96hr, Cyprinodon variegatus (Heitmuller et al. 1981) 96hr, Pimephales promelas (Pearson et al. 1979)
Other information about water organisms	Toxicity threshold (cell mult iplication inhibition test): green algae (Scenedesmus quadricauda): 0.83 mg/l protozoa (Entosiphon sulcatum): 5.9 mg/l (Bringmann & Kühn 1980a)	

914 • 2,4-Dinitrotoluene 121-14-2

Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 57 mg/l (Bringmann & Kühn 1980a).	
LOEC values to algae, mg/l	0.13	rpd, schr, Microcystis aeruginosa (Bringmann & Kuhn 1976)
EC50 values to crustaceans, mg/l	35	mbt, 48hr, Daphnia magna (Pearson et al. 1979)
LC50 values to fishes, mg/l	32.5	96hr, Pimephales promelas (Pearson et al. 1979)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 2.7 mg/l protozoa (Entosiphon sulcatum): 0.98 mg/l (Bringmann & Kühn 1980a)	

915 • 2,5-Dinitrotoluene 619-15-8

EC50 values to crustaceans, mg/l	3.4	mbt, 48hr, Daphnia magna (Pearson et al. 1979)
LC50 values to fishes, mg/l	1.3	96hr, Pimephales promelas (Pearson et al. 1979)

916 • 2,6-Dinitrotoluene 606-20-2

Use	Manufacturing TNT, urethane polymers, flexible and rigid foams and surface coatings and dyes; organic synthesis.	
Molecular weight	182.15	
Melting point, °C	64–66	
LD50 values to mammals in oral exposure, mg/kg	177 621	orl-rat orl-mus (Lewis & Sweet 1984)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 26 mg/l (Bringmann & Kühn 1980a)	
LOEC values to algae, mg/l	12	Scenedesmus quadricauda (Bringmann & Kühn 1980a)
EC50 values to crustaceans, mg/l	21.7	48hr, Daphnia magna (Pearson et al. 1979)
LC50 values to fishes, mg/l	19.8	96hr, Pimephales promelas (Pearson et al. 1979)
Other information about water organisms	LOEC 11 mg/l, rpd, schr, Entosiphon sulcatum (Bringmann & Kühn 1980a). EC50 100 mg/l, 24hr, rpd, Tetrahymena pyriformis (Yoshioka et al. 1985). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 12 mg/l protozoa (Entosiphon sulcatum): 11 mg/l (Bringmann & Kühn 1980a)	

917 • 3,4-Dinitrotoluene 610-39-9

Sumformula of the chemical	C7H6N2O4	
Molecular weight	182.15	
Water solubility, mg/l	100	(MITI 1992)
Melting point, °C	61	(MITI 1992)
Log octanol/water coefficient, log Pow	2.31	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.27 < 2.7	6w, Cyprinus carpio, conc 0.01 mg/l 6w, Cyprinus carpio, conc 0.001 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	

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LD50 values to mammals in oral exposure, mg/kg	177 747	orl-rat) orl-mus (Lewis & Sweet 1984
EC50 values to crustaceans, mg/l	3.1	mbt, 48hr, Daphnia magna (Pearson et al. 1979)
LC50 values to fishes, mg/l	1.5 1.8	96hr, Pimephales promelas (Pearson et al. 1979) 48hr, Oryzias latipes (MITI 1992)

918 • 3,5-Dinitrotoluene 618-85-9

Synonyms	1-Methyl-3,5-dinitrobenzene	
Sumformula of the chemical	C7H6N2O4	
Molecular weight	182.15	
LD50 values to mammals in oral exposure, mg/kg	216 607	orl-rat orl-mus (Lewis & Sweet 1984)
EC50 values to crustaceans, mg/l	45.1	mbt, 48hr, Daphnia magna (Pearson et al. 1979)
LC50 values to fishes, mg/l	22	96hr, Pimephales promelas (Pearson et al. 1979)

919 • Dinocap 6119-92-2

LOEC values to fishes, mg/l	0.02	srv, act, Salmo salar (Zitko et al. 1976)

920 • Dinonyl phthalate 84-76-4

Synonyms	1,2-Benzenedicarboxylic acid, dinonyl ester Phthalic acid, dinonyl ester	
LC50 values to crustaceans, mg/l	300	96hr, 21 °C, Nitocra spinipes (Linden et al. 1979)

921 • Dinonylnaphthalene sulfonate 25322-17-2

LC50 values to fishes, mg/l	10	50%, 96hr, Salmo gairdneri (Dave & Linman 1978)

922 • Dinoseb 88-85-7

Synonyms	2-(1-Methyl-n-propyl)-4,6-dinitrophenol 2,4-Dinitro-6-sec-butylphenol DNBP 2,4-Dinitro-6-(1-methylpropyl)phenol	
Use	Active ingredient in herbicides.	
State and appearance	Reddish brown liquid or dark brown solid.	
Molecular weight	240.24	
Vapour pressure, mmHg	1	151 °C
Water solubility, mg/l	25.8	(MITI 1992)

Log octanol/water coefficient, log Pow	4.074 3.09	(Anon. 1986) (MITI 1992)
Log soil sorption coefficient, log Kom	2.09	(Sabljic 1987)
Bioconcentration factor, fishes	< 0.3–1.0 < 2.5	6w, Cyprinus carpio, conc 0.01 mg/l 6w, Cyprinus carpio, conc 0.001 mg/l (MITI 1992)
LD50 values to mammals in oral exposure, mg/kg	25 20	orl-rat orl-mus (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	80	skn-rat (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	7 9 7.5 7.10–8.30	orl-bwd orl-dck (Lewis & Sweet 1984) orl-Agelaius phoeniceus orl-Sturnus vulgaris (Schafer et al. 1983)
Effects on plants	DNBP as the alkanolamine salt was applied to the leaf disks of tomato (Lycopersicon esculentum) either before, at the same time, or after incubation with p32 → 0.00000104 M (DNBP) for 3 hours of incubation inhibited p32 accumulation by 20%. (Wojtaszek et al. 1966). Germinated seedlings of pea (Pisum sativum) and barley (Hordeum vulgare) were grown in dinoseb-treated silica sand: 35 ppm dinoseb (as amine salt, in mg active material per litre solution; 12 ml of the solution was added to 225 g dry sand) caused 50% root inhibition over 72hr (O'Sullivan & Prendeville 1974).	
LC50 values to crustaceans, mg/l	0.68 1.8	act, Daphnia magna (Kenaga 1979) 96hr, Gammarus fasciatus (Sanders 1970)
LC50 values to fishes, mg/l	0.07–0.3 0.07 0.07 0.04–1.35 0.12 0.19 0.088 0.57	Salmo gairdneri (Kenaga 1979) 48hr, Cyprinus carpio 48hr, Carassius auratus (Hashimoto & Nishiuchi 1981) 96hr, Salmo clarci (Woodward 1976) 96hr, Ictalurus punctatus (McCorkle et al. 1977) 24hr, Oncorhynchus kisutch 144hr, O. kisutch (Lorz et al. 1979) 48hr, Oryzias latipes (MITI 1992)
LOEC values to fishes, mg/l	0.0005	grw, schr, Salmo trutta lacustris (Woodward 1976)

923 • N, N'-Dioctadecylurea

4051-66-5

Sumformula of the chemical	C37H76ON2	
Water solubility, mg/l	< 0.02	(MITI 1992)
Melting point, °C	107.2–114.0	(MITI 1992)
Bioconcentration factor, fishes	< 0.7–30 < 7.5–30	6w, Cyprinus carpio, conc 0.5 mg/l 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
LC50 values to fishes, mg/l	80.7	48hr, Oryzias latipes (MITI 1992)

D

D

924 • Dioctyl phthalate 117-84-0

Synonyms	Phthalic acid, dioctyl ester o-Benzenedicarboxylic acid, dioctyl ester 1,2-Benzenedicarboxylic acid, dioctyl ester Di-n-Octylphthalate Dioctyl o-benzenedicarboxylate
Sumformula of the chemical	C24H38O4
Molecular weight	390.62
Specific gravity (water=1)	0.99
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
Other information about degradation	Degradation of di-octyl-phthalate:

ENVIRONMENT	INIT. mg/l	REDOX-COND.	TEMP. °C	DEGRADATION %/day	REF.
water	5	aerobic	25	0/7	a
water	10	aerobic	25	0/7	a
water (adapt.)	5	aerobic	25	94/7	a
water (adapt.)	10	erobic	25	92/7	a
sludge	100	aerobic	30	48/20	b

a) Tabak et al. 1981 b) Engelhardt et al. 1977
(Anon. 1987b).

Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	6513	orl-mus (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	65000	ipr-mus (Sweet 1987)
TDLo values to mammals in oral exposure, mg/kg	78000	orl-mus, 7-14d preg effects on newborn (Sweet 1987)
TDLo values to mammals in non-oral exposure, mg/kg	5000	ipr-rat, 5-15d preg effects on embryo or fetus specific developmental abnormalities (Sweet 1987)
Health effects	Skin and eye irritation data: skin, rbt, 500 mg, 24hr, mild; eye, rbt, 5 mg, severe; eye, rbt, 500 mg, 24hr, mild (Sweet 1987).	

925 • Dioctyl sebacate 2432-87-3

Sumformula of the chemical	C26H50O4	
Melting point, °C	-55	(MITI 1992)
Boiling point, °C	248	/4 mmHg (MITI 1992)
Total degradation in water	Biodegradation: 78.2% by BOD period: 21d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

926 • Dioctyl tin maleate 16091-18-2

Synonyms	Di-n-octyltin maleate	
Water solubility, mg/l	< 10	(MITI 1992)
Melting point, °C	90–105	(MITI 1992)
Total degradation in water	Biodegradation: 3% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.4–1.6 < 3.9–9.1	6w, Cyprinus carpio, conc 2 mg/l 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	> 200	48hr, Oryzias latipes (MITI 1992)

927 • Dioxacarb 6988-21-2

Synonyms	2-(1,3-Dioxolan-2-yl)-phenylmethyl carbamate	
LD50 values to mammals in oral exposure, mg/kg	60 61 100	orl-rat orl-mus orl-mam (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	1660 3000	skn-mus skn-rat (Lewis & Sweet 1984)
LC50 values to fishes, mg/l	25.5 25.5 2.7	48hr, Cyprinus carpio Poecilia reticulata 48hr, Salmo gairdneri (Hejduk & Svobodova 1980)

928 • 1,3-Dioxane 505-22-6

Synonyms	m-Dioxane	
Molecular weight	88.12	
Melting point, °C	-42	
Boiling point, °C	105	
Maximum longterm immission concentration in air for plants, mg/m³	20	VDI 2306
Maximum longterm immission concentration in air for plants, ppm	5	VDI 2306

929 • 1,4-Dioxane

123-91-1

Synonyms	p-Dioxane Diethylene ether Diethylene dioxide 1,4-Diethylene dioxide 1,4-Dioxacyclohexane Dioxyethylene ether Glycol ethylene ether Tetrahydro-p-dioxin
Sumformula of the chemical	C4H8O2
Use	Solvent for cellulosics and wide range of organic products; lacquers; paints; varnish.
Odour	Quality: sweet, alcohol Hedonic tone: pleasant Threshold odour concentration absolute: 0.80 ppm 50% recognition: 1.8 ppm 100% recognition: 5.7 ppm Odour index 100% recognition: 6 228 (Hellman & Small 1974).
Molecular weight	88.12
Vapour pressure, mmHg	30 20 °C
Melting point, °C	10.0–11.9 (MITI 1992)
Boiling point, °C	101
Henry's law constant, Pa x m³/mol	0.6964 calc. (Yaws et al. 1991)
Volatilization	Relative volatility (nBuAc=1) = 2.72
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Bioconcentration factor, fishes	0.2–0.6 6w, Cyprinus carpio, conc 10 mg/l 0.3–0.7 6w, Cyprinus carpio, conc 1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	4200 orl-rat 2000 orl-cat, orl-rbt (Lewis & Sweet 1984) 3150 orl-gpg 5700 orl-mus (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	7600 skn-rbt (Lewis & Sweet 1984) 790 ipr-mus 5600 ipr-rat (Sweet 1987)

LC50 values to mammals in inhalation exposure, mg/m³	65000 46000	2hr, ihl-mus 2hr, ihl-rat (Sweet 1987)
LDLo values to mammals in non-oral exposure, mg/kg	1500 1500	ivn-cat ivn-rbt (Sweet 1987)
LCLo values to mammals in inhalation exposure, mg/kg	44000	ihl-cat, 7hr (Sweet 1987)
LCLo values to mammals in inhalation exposure, ppm	470	3d, ihl-hmn (Lewis & Sweet 1984)
TDLo values to mammals in oral exposure, mg/kg	10000 239000 185000	orl-rat, 6-15d preg. effects on embryo or fetus specific developmental abnormalities (Sweet 1987) orl-mus, tumorigenic orl-rat, tumorigenic (Sweet 1987)
TDLo values to mammals in non-oral exposure, mg/kg	12000 14000	ipr-mus, tumorigenic skn-mus, tumorigenic (Sweet 1987)
TCLo values to mammals in inhalation exposure, ppm	111 470 5500	ihl-rat, tumorigenic (Sweet 1987) ihl-hmn ihl-hmn, 1 min (Sweet 1987)
Other information about mammals	Skin and eye irritation data: eye, human, 300 ppm, 15 min; skin, rabbit, 515 mg open, mild; eye, rabbit, 21 mg; eye, guinea pig, 0.010 mg, moderate (Sweet 1987).	
Carcinogenicity	NCI carcinogenesis bioassay (oral); clear evidence: mouse, rat (Sweet 1987).	
Mutagenicity	Mutation data: DNA damage: rat, liver, 0.3 mmol/l; unscheduled DNA synthesis: rat, oral; 20 mg/kg; test systers (other): rat, intravenous, 50 mg/kg (Sweet 1987).	
LOEC values to algae, mg/l	575	rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to fishes, mg/l	6700 10500	96hr, Menidia audens (Dawson et al. 1977) 48hr, Oryzias latipes (MITI 1992)

930 • Dioxathion

78-34-2

Synonyms	1,4-Diocane-2,3-diyl-bis-diethylphosphorodithioate
Use	Insecticide.
State and appearance	Brown liquid.
Molecular weight	456.56

LD50 values to mammals in oral exposure, mg/kg	20 orl-rat 10 orl-dog (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	63 skn-rat 85 skn-rbt (Lewis & Sweet 1984)
Carcinogenicity	NCI carcinogenesis bioassay completed: results negative; mus, rat (Lewis & Sweet 1984).
LD50 values to birds in oral exposure, mg/kg	170 orl-ckn (Lewis & Sweet 1984) > 100 orl-Agelaius phoeniceus (Schafer et al. 1983)
LC50 values to crustaceans, mg/l	0.0086 96hr, Gammarus fasciatus (Sanders 1972)
LC50 values to fishes, mg/l	0.034 96hr, Lepomis macrochirus 0.036 96hr, Micropterus salmoides (Pickering et al. 1962)

931 • 1,3-Dioxolan-2-on 96-49-1

Synonyms	1,3-Dioxolane-2-one
Melting point, °C	36.3 (MITI 1992)
Boiling point, °C	238 (MITI 1992)
Total degradation in water	Biodegradation: 64.1% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

932 • Dipentamethylene thiuramtetrasulfide 120-54-7

Synonyms	Piperidine, 1,1'-(tetrathiodicarbonothioyl)bis-
Sumformula of the chemical	C12H20N2S6
EINECS-number	2044060
Water solubility, mg/l	< 10 (MITI 1992)
Log octanol/water coefficient, log Pow	2.8 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	1.0–10 6w, Cyprinus carpio, conc 0.5 mg/l < 1.9–32 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 500 48hr, Oryzias latipes (MITI 1992)

933 • Dipentyl ketone 927-49-1

Sumformula of the chemical	C11H22O
Water solubility, mg/l	50 (MITI 1992)
Melting point, °C	14–15 (MITI 1992)
Boiling point, °C	226 (MITI 1992)
Total degradation in water	Biodegradation: 55–86% by BOD (on the upward trend) period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

934 • Diphenyl ether 101-84-8

Synonyms	Diphenyloxide phenoxybenzone Phenylether	
Sumformula of the chemical	C12H10O	
Use	Organic synthesis; perfumery, particularly soaps; heat transfer medium.	
State and appearance	Colourless liquid.	
Molecular weight	170.22	
Vapour pressure, mmHg	0.02	25 °C
Water solubility, mg/l	21	25 °C
Melting point, °C	26.7	(MITI 1992)
Boiling point, °C	259	(MITI 1992)
Log octanol/water coefficient, log Pow	4.21 4.21 4.21 4.21	(Anon. 1986) (Mackay 1982) (Hawker & Connell 1985) (Sangster 1989)
Total degradation in water	Biodegradaion: 6.3% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	195 112–583 49–594	Salmo gairdneri (Verschueren 1983) 8w, Cyprinus carpio, conc 0.3 mg/l 8w, Cyprinus carpio, conc 0.03 mg/l (MITI 1992)
LD50 values to mammals in oral exposure, mg/kg	3370	orl-rat (Lewis & Sweet 1984)
LC50 values to crustaceans, mg/l	0.67	48hr, Daphnia magna (LeBlanc 1980)
LC50 values to fishes, mg/l	2.4 4 4.6	96hr, Cyprinodon variagetus (Heitmuller et al. 1981) 96hr, Pimephales promelas (Veith et al. 1983) 48hr, Oryzias latipes (MITI 1992)

935 • N, N-Diphenyl guanidine 102-06-7

Synonyms	1,3-Diphenylguanidine N, N'-Diphenylguanidine	
Water solubility, mg/l	0.1 g/100 g (25 °C) (MITI 1992)	
Melting point, °C	149.0–150.0 (MITI 1992)	
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).	
Bioconcentration factor, fishes	< 2 < 20	6w, Cyprinus carpio, conc 0.1 mg/l 6w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LD50 values to birds in oral exposure, mg/kg	> 100 > 100	orl-Agelaius phoeniceus orl-Passer domesticus (Schafer et al. 1983)
LC50 values to fishes, mg/l	10	48hr, Oryzias latipes (MITI 1992)

936 • Diphenyl methane 101-81-5

Sumformula of the chemical	C13H12	
Water solubility, mg/l	< 10	(MITI 1992)
Melting point, °C	26–27	(MITI 1992)
Boiling point, °C	261–262	(MITI 1992)
Log octanol/water coefficient, log Pow	4.14 4.49	(Sangster 1989) (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	452–1150 536–1190	8w, Cyprinus carpio, conc 0.1 mg/l 8w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be accumulated on a medium level (Anon. 1987).	
LC50 values to fishes, mg/l	2.76	48hr, Oryzias latipes (MITI 1992)

937 • Diphenyl methanol 91-01-0

Sumformula of the chemical	C13H120	
Water solubility, mg/l	600	(MITI 1992)

Melting point, °C	64–67 (MITI 1992)
Boiling point, °C	297–298, 748 mmHg (MITI 1992)
Log octanol/water coefficient, log Pow	2.67 (Sangster 1989)
Total degradation in water	Biodegradation: 51–100% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

938 • 2,2'-Diphenyl-2-hydroxy acetic acid 76-93-7

Water solubility, mg/l	> 1000	(MITI 1992)
Melting point, °C	149.8	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.2 < 1.8	6w, Cyprinus carpio, conc 1 mg/l 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	365	48hr, Oryzias latipes (MITI 1992)

939 • N, N'-Diphenyl-p-phenylenediamine 74-31-7

Sumformula of the chemical	C18H16N2	
EINECS-number	2008064	
Water solubility, mg/l	< 10	(MITI 1992)
Melting point, °C	> 130	(MITI 1992)
Total degradation in water	Biodegradation: 0.2% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	264–1418 495–2146	8w, Cyprinus carpio, conc 0.1 mg/l 8w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
LC50 values to fishes, mg/l	36	48hr, Oryzias latipes (MITI 1992)

940 • Diphenylamine 122-39-4

Sumformula of the chemical	C12H11N	
Melting point, °C	54	(MITI 1992)
Boiling point, °C	302	(MITI 1992)
pKa	0.78	(Sangster 1989)
Log octanol/water coefficient, log Pow	3.4 3.42 3.5	(Anon. 1986) (Mackay 1982) (Sangster 1989)
Log soil sorption coefficient, log Kom	2.54	(Sabljic 1987)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).	
Bioconcentration factor, fishes	101–242 51–253	8w, Cyprinus carpio, conc 0.1 mg/l 8w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LD50 values to birds in oral exposure, mg/kg	> 101	orl-Agelaius phoeniceus (Schafer et al. 1983)
LC50 values to fishes, mg/l	5.1	48hr, Oryzias latipes (MITI 1992)

941 • 1,2-Diphenylhydrazine 122-66-7

LC50 values to crustaceans, mg/l	4.1	48hr, Daphnia magna (LeBlanc 1980)
LC50 values to fishes, mg/l	0.27	96hr, Lepomis macrochirus (Buccafusco et al. 1981)

942 • Diphenylmonotridecylphosphite 60628-17-3

Sumformula of the chemical	C25H37O3P	
Melting point, °C	-10	(MITI 1992)
Total degradation in water	Biodegradation: 14–25% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 11 < 113	6w, Cyprinus carpio, conc 0.1 mg/l 6w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
LC50 values to fishes, mg/l	291	48hr, Oryzias latipes (MITI 1992)

943 • Diphenyltin dichloride 1135-99-5

LC50 values to algae, mg/l	0.031 72hr, Skeletonema costatum (Walsh et al. 1985)

944 • Dipotassium octylphosphate and potassium dioctylphosphate 19045-79-5

Sumformula of the chemical	C8H17O4PK2; C16H34O4PK
Water solubility, mg/l	> 2500 (MITI 1992)
Total degradation in water	Biodegradation: 57–92% by BOD (on the upward trend) period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

945 • Dipropylenglycol 110-98-5

Synonyms	Bis(3-hydroxypropyl)ether
Sumformula of the chemical	C6H14O3
Use	Polyester and alkyd resins, reinforced plastics, plasticizers, solvent.
State and appearance	Water-white liquid. Odour: Amine odour.
Water solubility, mg/l	100000 (MITI 1992)
Melting point, °C	< -10 (MITI 1992)
Boiling point, °C	230–235 (MITI 1992)
Flashing point, °C	137.7 open cup
Other physicochemical properties	Combustible
Chemical oxygen demand, g O2/g	1.84 5 days (Bridie et al. 1979)
Biochemical oxygen demand, g O2/g	0.09 5 days (Bridie et al. 1979)
Total degradation in water	Biodegradation: 0–3% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).
Bioconcentration factor, fishes	0.3–1.4 6w, Cyprinus carpio, conc 3 mg/l < 2.2–4.6 6w, Cyprinus carpio, conc 0.3 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 5000 24hr, Carassius auratus (Bridie et al. 1979) > 1000 48hr, Oryzias latipes (MITI 1992)

946 • Dipropylphthalate 131-16-8

Synonyms	DPP	
LC50 values to algae, mg/l	1.3–6.5	96hr, Gymnodium breve (EPA 1975)
EC50 values to algae, mg/l	0.9–2.4	rpd, act, Gymnodium breve (EPA 1975)

947 • Direct Black-154 37372-50-2

Water solubility, mg/l	> 5000	(MITI 1992)
Log octanol/water coefficient, log Pow	-1.67	(MITI 1992)
Bioconcentration factor, fishes	8.1–22 39–66	8w, Cyprinus carpio, conc 1 mg/l 8w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
LC50 values to fishes, mg/l	135	48hr, Oryzias latipes (MITI 1992)

948 • Direct Yellow-86 50925-42-3

Water solubility, mg/l	> 25000	(MITI 1992)
Bioconcentration factor, fishes	< 0.6–1.8 < 5.5	6w, Cyprinus carpio, conc 2 mg/l 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 1000	48hr, Oryzias latipes (MITI 1992)

949 • Disodium arsenate 7778-43-0

Synonyms	Arsenic acid, disodium salt Disodium arsenic acid Sodiumhydrogen arsenate Disodium hydrogen orthoarsenate Disodiummono–hydrogen arsenate Sodium arsenate Sodium acid arsenate	
Sumformula of the chemical	AsHO4Na2	
Molecular weight	185.91	
Bioconcentration factor, algae	10000	arsenate, blue-green algae, dry weight (Blanck et al. 1989)
LDLo values to mammals in non-oral exposure, mg/kg	30	ipr-rat (Lewis & Sweet 1984)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 18 mg/l (Bringmann & Kühn 1980a)	
EC50 values to algae, mg/l	0.006	As, arsenate, periphyton, pht, southern Baltic sea (Blanck et al. 1989)
LOEC values to algae, mg/l	 0.0007–0.008 0.0002—0018 0.023	arsenate mg As/l, phytoplankton pht, oligotrophic lake mg As/l, periphyton pht, oligotrophic lake (Wängberg 1989) As, periphyton, Skagerak, pht (Blanck et al. 1989)

LC50 values to crustaceans, mg/l	0.005-0.008 mg As/l, arsenate, Fucus vesiculosus (Notini et al. 1987)	
LC50 values to fishes, mg/l	49	96hr, Gambusia affinis (Jurewicz & Buikema 1980)
	100	As, arsenate, 48hr, Lepomis (Sorensen 1976)
Other information about water organisms	LOEC, 0.02 mg As/l, rpd, Pontoporeia, Baltic Sea; LOEC, 0.023–0.075 mg As/l, Capitella, egg production, Skagerak (Blanck et al. 1989). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 8.7 mg/l protozoa (Entosiphon sulcatum): 8.9 mg/l (Bringmann & Kühn 1980a)	

950 • Disodium-2-naphthol-3,6-disulfonate 135-51-3

Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).

951 • Disperse Blue-143 61968-28-3

Melting point, °C	153	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BODF period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	0.51–4.41 3.3–5.0	6w, Cyprinus carpio, conc 0.6 mg/l 6w, Cyprinus carpio, conc 0.06 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	> 60	48hr, Oryzias latipes (MITI 1992)

952 • Disperse Blue 54 12217-77-5

Sumformula of the chemical	C20H12O6N2	
Water solubility, mg/l	> 10	(MITI 1992)
Melting point, °C	185–195	(MITI 1992)
Log octanol/water coefficient, log Pow	4.68	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	5.6–9.2 14–25	6w, Cyprinus carpio, conc o.2 mg/l 6w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 100	48hr, Oryzias latipes (MITI 1992)

953 • Disperse Orange 73 40690-89-9

Water solubility, mg/l	> 10 (MITI 1992)
Melting point, °C	147–153 (MITI 1992)
Log octanol/water coefficient, log Pow	> 5.4 (MITI 1992)
Total degradation in water	Biodegradation: 3–11% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	0.8–14 6w, Cyprinus carpio, conc 0.1 mg/l < 2.5–11 6w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 50 48hr, Oryzias latipes (MITI 1992)

D

954 • Disperse Red 167 61968-52-3

Water solubility, mg/l	< 10 (MITI 1992)
Melting point, °C	145–150 (MITI 1992)
Log octanol/water coefficient, log Pow	4.53 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.3–1.1 6w, Cyprinus carpio, conc 0.1 mg/l < 3.3–7.4 6w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 100 48hr, Oryzias latipes (MITI 1992)

955 • Disperse Red 206 26630-87-5

Water solubility, mg/l	< 10 (MITI 1992)
Melting point, °C	142.1–144.5 (MITI 1992)
Log octanol/water coefficient, log Pow	> 6 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	2.0–6.6 6w, Cyprinus carpio, conc 0.2 mg/l 8.0–25 6w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 500 48hr, Oryzias latipes (MITI 1992)

956 • Disperse Red 207

59722-76-8

Sumformula of the chemical	C20H12O4NBr
Water solubility, mg/l	> 10 (MITI 1992)
Melting point, °C	215–218.2 (MITI 1992)
Log octanol/water coefficient, log Pow	> 5.5 (MITI 1992)
Total degradation in water	Biodegradation: 0–1% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	9.2–48 8w, Cyprinus carpio, conc 0.2 mg/l 46–178 8w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 100 48hr, Oryzias latipes (MITI 1992)

957 • Disperse Yellow 163

71767-67-4

Sumformula of the chemical	C18H14O2N6Cl2
Water solubility, mg/l	< 0.00066 (MITI 1992)
Melting point, °C	189.5–190.5 (MITI 1992)
Log octanol/water coefficient, log Pow	4.19 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	30–49 6w, Cyprinus carpio, conc 0.1 mg/l 26–47 6w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 100 48hr, Oryzias latipes (MITI 1992)

958 • Disperse Yellow 42

5124-25-4

Sumformula of the chemical	C18H15O4N2S
Water solubility, mg/l	< 10 (MITI 1992)
Melting point, °C	155–157.6 (MITI 1992)
Log octanol/water coefficient, log Pow	4.37 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

Bioconcentration factor, fishes	17–30 33–48	6w, Cyprinus carpio, conc 0.5 mg/l 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 250	48hr, Oryzias latipes (MITI 1992)

959 • Disperse Yellow 64

10319-14-9

Water solubility, mg/l	< 10	(MITI 1992)
Melting point, °C	262–264	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	0.82–27 < 1.4–4.9	6w, Cyprinus carpio, conc 0.2 mg/l 6w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	> 100	48hr, Oryzias latipes (MITI 1992)

960 • Distamycin A

636-47-5

Other information about mammals	LDfr = 75.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).	
LD50 values to birds in oral exposure, mg/kg	< 72	orl-Agelaius phoeniceus (Schafer et al. 1983)

961 • Distearylthio dipropionic ester

693-36-7

Synonyms	Distearyl thiodi ester propionate	
Melting point, °C	65	(MITI 1992)
Boiling point, °C	250	1 mmHg (MITI 1992)
Total degradation in water	Biodegradation: 51% by BOD (on the upward trend) period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	

962 • Disulfoton

298-04-4

Synonyms	0,0-Diethyl-S-(2-(ethylthio)ethyl)phosphorodithioate
Use	Acaricide, insecticide.
State and appearance	Pale yellow liquid.

Molecular weight	274.42	
Vapour pressure, mmHg	1.8	20 °C
Water solubility, mg/l	25	
Boiling point, °C	62	
Log soil sorption coefficient, log Kom	3.25	(Sabljic 1987)
Half-life in soil, days	5	(Li et al. 1990)
LD50 values to mammals in oral exposure, mg/kg	2 5.5	orl-rat orl-mus (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	6	skn-rat (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	6.5 3.2 3.16 > 31.6 2.37	orl-dck orl-bwd (Lewis & Sweet 1984) orl-Agelaius phoeniceus orl-Sturnus vulgaris orl-Quiscalus quiscula (Schafer et al. 1983)
LC50 values to crustaceans, mg/l	0.021	96hr, Gammarus fasciatus (Sanders 1972)
LC50 values to fishes, mg/l	0.04 3.02 4 0.063 0.0014	act, Salmo gairdneri (Kenaga 1979) 96hr, Salmo gairdneri (Holcombe et al. 1982) 96hr, Pimephales promelas (Holcombe et al. 1982) 96hr, Lepomis macrochirus (Pickering et al. 1962) 30d, Acroneurica pacifica (Jensen & Gaufin 1964)
Other information about water organisms	LC50 30d, 0.0014 mg/l, Acroneuria pacifica (Jensen & Gaufin 1964)	

963 • Diuron

330-54-1

Synonyms	3-(3,4-Dichlorophenyl)-1,1-dimethylurea N'-(3,4-Dichlorophenyl)-N,N-dimethylurea DMU DCMU	
Use	Herbicide.	
Molecular weight	233.11	
Vapour pressure, mmHg	0.0000031 50 °C	
Water solubility, mg/l	42 34	25 °C (MITI 1992)
Melting point, °C	156–158	(MITI 1992)
Log octanol/water coefficient, log Pow	2.96	(MITI 1992)
Log soil sorption coefficient, log Kom	1.97	(Sabljic 1987)
Half-life in soil, days	328	(Li et al. 1990)

Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	3.4–4.9 < 2.9–14	6w, Cyprinus carpio, conc 0.5 mg/l 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
LD50 values to mammals in oral exposure, mg/kg	1017	orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	3400	unk-rat (Lewis & Sweet 1984)
Effects on arthropods	LC50 1.2 mg/l, 96hr, mosquito (Knapek & Lakola 1974).	
Effects on plants	Germinated and fungicide-treated barley (Hordeum vulgare L.) seeds were sown to sandy loam soil -> first significant depression of top growth occurred at 0.4 kg diuron/ha. This was associated with some toxicity symptoms such as paleing and leaf-tip dieback (Toth & Milham 1975). Germinated seedlings of pea (Pisum sativum) and barley (Hordeum vulgare) were grown in diuron-treated silica sand: 160 ppm diuron (in mg active material per litre solution; 12 ml of the solution was added to 225 g dry sand) caused 50% root inhibition over 72hr (O'Sullivan & Prendeville 1974).	
EC50 values to algae, mg/l	0.01	10d, pht, Dunaliella terticulata Isochyris galbana Phaeodactylum tricornutum (Walsh 1972)
LC50 values to crustaceans, mg/l	0.16	96hr, Gammarus lacustris (Sanders 1969)
	1.4	48hr, Daphnia pulex, Sanders & Cope 196
	1.4	24hr, Daphnia magna (Frear & Boyud 1967)
	0.4	96hr, Daphnia magna (Knapek & Lakola 1974)
	40	act, Daphnia pulex (Nishiuchi & Hashimoto 1967)
	47	act, Daphnia magna (Kenaga 1979)
LC50 values to fishes, mg/l	16	48hr, Oncorhynchus kisutch (Bond et al. 1960)
	7.4 4.3	48hr, Lepomis macrochirus 48hr, Salmo gairdneri (Edwards 1977)
	2.9	96hr, Cyprinus carpio (Knapek & Lakola 1974)
	3.2	48hr, Cyprinus carpio (Nishiuchi & Hashimoto 1967)
	5.9 3–60	act, Lepomis macrochirus act, Salmo gairdneri (Kenaga 1979)
	23.3 7.7	1d, Pimephales promelas 8d, Pimephales promelas (Call et al. 1987)
	> 100	48hr, Oryzias latipes (MITI 1992)
Other information about water organisms	Aquatic community; EC50, 4d, 2.205 mg/l (Flum & Shannon 1987).	

964 • m-(or p-)Divinylbenzene 1321-74-0

Sumformula of the chemical	C10H11	
Water solubility, mg/l	20 8.2	m- (MITI 1992) p- (MITI 1992)
Boiling point, °C	52 52	3 mmHg, m- (MITI 1992) 3 mmHg, p- (MITI 1992)
Log octanol/water coefficient, log Pow	4.15 4.18	m- (MITI 1992) p- (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	219–415 206–402 264–444 229–385	6w, Cyprinus carpio, conc 0.025 6w, Cyprinus carpio, conc 0.025 mg/l 6w, Cyprinus carpio, conc 0.0025 mg/l 6w, Cyprinus carpio, conc 0.0025 mg/l (MITI 1992)
LC50 values to fishes, mg/l	3.45	48hr, Oryzias latipes (MITI 1992)

965 • n-Docosane 629-97-0

LC50 values to crustaceans, mg/l	> 530	48hr, Daphnia magna (LeBlanc 1980)

966 • 13-Docosenamide 112-84-5

Synonyms	cis-13-Docosenoic acid amide	
Water solubility, mg/l	< 10 mg/l	(MITI 1992)
Melting point, °C	81.5	(MITI 1992)
Boiling point, °C	205	1 mmHg (MITI 1992)
Total degradation in water	Biodegradation: 85–91% by BOD period: 21d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	

967 • Dodecachloro dodecahydro dimethanodibenzo cyclooctene 13560-89-9

Synonyms	1,4:7,10-Dimethanodibenzo(a, e)cyclooctene, 1,2,3,4,7,8,9,10,13,13,14,14 -dodecachloro-1,4,4a,5,6,6a,7,10,10a,11,12,12a-dodecahydro-
Sumformula of the chemical	C18H12Cl12
EINECS-number	2369489

Melting point, °C	> 350 (MITI 1992)
Total degradation in water	Biodegradation: 0.6% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Bioconcentration factor, fishes	23–121 8w, Cyprinus carpio, conc 0.00265 mg/l 14–96 8w, Cyprinus carpio, conc 0.00027 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).

D

968 • 1,12-Dodecanedicarboxylic acid 821-38-5

Sumformula of the chemical	$C_{14}H_{26}O_4$	
Water solubility, mg/l	2	(MITI 1992)
Melting point, °C	126.0–127.5	(MITI 1992)
Total degradation in water	Biodegradation: 86–93% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

969 • Dodecanoic acid 143-07-7

Synonyms	Lauric acid	
Sumformula of the chemical	$C_{12}H_{24}O_2$	
Use	Alkyl resins, wetting agents, soaps, detergents, cosmetics, insecticides, food additives.	
State and appearance	Colourless needles.	
Specific gravity (water=1)	0.833	
Melting point, °C	44	
Boiling point, °C	225	100 mm
pKa	5.3	(Sangster 1989)
Log octanol/water coefficient, log Pow	4.2 4.6	(Anon. 1986) (Sangster 1989)
Other physicochemical properties	Insoluble in water, soluble in benzene and ether.	

970 • 1-Dodecanol 112-53-8

Synonyms	Dodecyl alcohol
Sumformula of the chemical	$C_{12}H_{26}O$

Log octanol/water coefficient, log Pow	5.13	(Sangster 1989)
Henry's law constant, Pa x m³/mol	9.125	calc. (Yaws et al. 1991)
LC50 values to crustaceans, mg/l	0.9	96hr, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	1.01	96hr, Pimephales promelas (Veith et al. 1983)

971 • Dodecenylsuccinic anhydride 25377-73-5

Synonyms	1-Dodecen-2-ylsuccinic acid anhydride	
Sumformula of the chemical	C16H2603	
Chemical oxygen demand, g 02/g	2.44	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	1.02	5 days (Bridie et al. 1979)
LC50 values to fishes, mg/l	4	24hr, Carassius auratus (Bridie et al.1979)

972 • 4-Dodecylaniline 104-42-7

Sumformula of the chemical	C18H31N	
EINECS-number	2032013	
Water solubility, mg/l	< 10	(MITI 1992)
Melting point, °C	41–42	(MITI 1992)
Boiling point, °C	220–221	15 mmHg (MITI 1992)
Total degradation in water	Biodegradation: 42–76% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	

973 • Dodecylbenzenesulfonate 1886-81-3

Effects on the physiology of water organisms	Cyprinus carpio; 7.2 mg/l, 0.17d, biochemical effect (change in physiochemical process including glycogen uptake, cholesterol levels and lipid analysis) (Nakanishi et al. 1986).

974 • Dodecylguanidine acetate 2439-10-3

Synonyms	n-Dodecylguanidine acetate Dodine Dodine acetate Laurylguanidine acetate Syllit Venturol
Sumformula of the chemical	C15H3302N3

Molecular weight	287.51	
LD50 values to mammals in oral exposure, mg/kg	566 1200	orl-rat orl-mus (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	1000 1500	unk-rat skn-rbt (Lewis & Sweet 1984)
TDLo values to mammals in non-oral exposure, mg/kg	1000	scu-mus (Lewis & Sweet 1984)
Other information about mammals	ALD = 94.0 mg/kg, act, orl, deer mouse; LDfr = 62.5 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).	
LC50 values to fishes, mg/l	0.6	96hr, Rasbora heteromospha (Tooby et al. 1975)

D

975 • p-Dodecylphenol 27193-86-8

LC50 values to fishes, mg/l	0.14	96hr, Salmo clarci (McLeese et al. 1981)

976 • Dodecyltrimethylammonium chloride 112-00-5

Other information about water organisms	Poteriochromonas malhamensis; 8.98 mg/l, 3d, 0% survival or 100% mortality including algicidal and herbicidal effects (Roderer 1987).

977 • Donax 87-52-5

LC50 values to fishes, mg/l	1050	24hr, Carassius auratus (Anon. 1975)

978 • Dowco 160 35944-82-2

Other information about mammals	LDfr = 75.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).	
LD50 values to birds in oral exposure, mg/kg	10 17.8 5.62	orl-Agelaius phoeniceus orl-Sturnus vulgaris orl-Passer domesticus (Schafer et al. 1983)

979 • Dowicide A * 132-27-4

Use	Manufacture of fungicides.	
EC50 values to algae, mg/l	25	10d, pht, Protococcus sp. Phaeodactylum tricornutum Monochrystis lutheri (Ukeles 1962)

980 • Eicosane 112-95-8

Sumformula of the chemical	C20H42
EINECS-number	2040181

Water solubility, mg/l	1 (MITI 1992)
Melting point, °C	36.5 (MITI 1992)
Boiling point, °C	205 15mmHg (MITI 1992)
Henry's law constant, Pa x m³/mol	32.73 calc. (Yaws et al. 1991)
Total degradation in water	Biodegradation: 89% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

981 • Endosulfan

115-29-7

Synonyms	6,7,8,9,10-Hexachloro-1,5,5a,6,9,9a-hexahydro-6,9-methano-2,4,3 -benzodioxathiepin-3-oxide	
Products containing the chemical	Chlorthiepin Malix Thiodan	
Use	Active ingredient in insecticides; acaricide.	
State and appearance	Brown crystals.	
Molecular weight	406.91	
Melting point, °C	70–100	
Total degradation in water	0% of original compound found after 4 weeks in river water (initial concentration 10 µg/l) (Verschueren 1983).	
Bioconcentration factor, fish	620–1344	(Verschueren 1983)
Bioconcentration factor, mollusca	600	Mytilus edulis (Verschueren 1983)
Bioconcentration factor, crustaceans	81–245	Palaemonetes pugio (Verschueren 1983)
LD50 values to mammals in oral exposure, mg/kg	18 2 7.36	orl-rat orl-cat orl-mus (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	74 100	skn-rat (Lewis & Sweet 1984) ukn-rat (Virtanen & Nuuja 1987)
LD50 values to birds in oral exposure, mg/kg	33 35 35	orl-dck orl-bwc (Lewis & Sweet 1984) orl-Sturnus vulgaris (Schafer et al. 1983)
LC50 values to crustaceans, mg/l	0.06 0.00004 0.158–0.740 0.0108 0.24 0.00352	48hr, Daphnia magna (Sanders & Cope 1966) 96hr, Penaeus duorarum (Verschueren 1983) 48hr, Daphnia magna (Nebeker 1982) 96hr, Saccobranchus fossilis (Verma et al. 1982) act, Daphnia pulex (Frear & Boyd 1967) 96hr, Macrobrachium lamarrei (Shukla & Omkar 1984)

EF

NOEC values to crustaceans, mg/l	0.003	rpd, schr, Daphnia magna (Macek et al. 1976c)
LC50 values to fishes, mg/l	0.0003	96hr, Salmo gairdneri (Schoettger 1970, Macek et al. 1976a)
	0.00009	96hr, Leistomus canthurus (Schoettger 1970)
	0.0015	96hr, Fundulus heteroclitus (Trim 1987)
	0.0015	24hr, Cyprinus carpio (Hashimoto et al.1982)
	0.004	act, Barbus stigma (Manoharan & Subbiah 1982)
	0.002	96hr, Heteropneustes fossilis (Singh & Srivastava 1982)
	0.0027	96hr, Poecilia reticulata (Gupta et al. 1984)
	0.0097	96hr, Heteropneustes fossilis (Singh & Narain 1982)
	0.0003	96hr, Salmo gairdneri (Macek et al. 1976)
	0.020–0.042	4d, Anguilla anguilla (Ferrando et al. 1987)
	0.006308–0.008689 0.000891–0.003199 0.001711–0.004078 0.001331–0.004302 0.000261–0.002428 0.001387–0.004341 0.000356–0.002688	4d Barbus javanicus 4d Catla catla 4d Ctenopharyngodon idella 1d Hypophthalmichthys molitrix 4d Hypophthalmichthys molitrix 1d Labeo rohita 4d Labeo rohita (Paul & Raut 1987)
	0.00205–0.00328	4d Tilapia aurea (Herzberg 1986)
LOEC values to fishes, mg/l	0.0004	rpd, chr, Pimephales promelas (Macek et al. 1976c)
NOEC values to fishes, mg/l	0.0002	rpd, chr, Pimephales promelas (Macek et al. 1976c)
Effects on the physiology of water organisms	Oziotelphusa senex senex; 3.8 mg/l, 4d, biochemical effect (change in physiochemical process including glycogen uptake, cholesterol levels and lipid analysis) (Vijayakumari et al. 1987). Oziotelphusa senex senex; 3.8 mg/l, 4d, change in enzyme activity (Naidu et al. 1986).	
Other information about water organisms	Procambarus clarkii; 0.560 mg/l, 4d, 100% mortality or 0% surviving including algicidal and herbicidal effects (Andreu-Moliner et al. 1986).	
	LC50, > 1.89 mg/l, 96hr, renewal, Aplexa hypnorum (Holcombe et al. 1983)	

982 • Endosulfan A 959-98-8

Use	Insecticide.
LC50 values to fishes, mg/l	0.00016 96hr, Channa punctata, Devi et al.1981

983 • Endosulfan B 33213-65-9

Use	Insecticide.
LC50 values to fishes, mg/l	66 act, Channa punctata (Devi et al.1981)

984 • Endothal 129-67-9

Synonyms	7-Oxabicyclo(2,2,1)heptane-2,3-dicarboxylic acid, disodium salt
Sumformula of the chemical	C8H8O5 .2Na
Use	Herbicide.

Molecular weight	230.14	
LD50 values to mammals in oral exposure, mg/kg	51	orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	750 5	skn-rat (Lewis & Sweet 1984) ivn-dog (Lewis & Sweet 1984)
LDLo values to mammals in oral exposure, mg/kg	250	orl-gpg (Lewis & Sweet 1984)
LDLo values to mammals in non-oral exposure, mg/kg	5	ivn-rbt (Lewis & Sweet 1984)
Other information about mammals	In diet: Endothal-Na, fed for 2 years to rats at 1000 ppm caused no ill effects (Martin 1968).	
LC50 values to fishes, mg/l	110 125 120 200 95 136	96hr, Pimephales notatus 96hr, Lepomis macrochirus 96hr, Micropterus salmoides 96hr, Micropterus salmoides 96hr, Notropis umbratilus 96hr, Oncorhynchus tschawtscha (Walker 1964)

985 • Endrin

72-20-8

Synonyms	1,2,3,4,10,10-Hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a-octa-hydroexo-1,4-exo-1,4-exo-5,8-dimethanonaphthalene	
Use ceased in year	1979	
Use	Insecticide, rodenticide.	
Molecular weight	380.9	
Vapour pressure, mmHg	0.0000002 25 °C	
Water solubility, mg/l	0.18	(MITI 1992)
Melting point, °C	200 245	approx. 200 (MITI 1992)
Log octanol/water coefficient, log Pow	5.63 4.56 5.22	(Anon. 1988) (Mackay 1982) (MITI 1992)
Henry's law constant, Pa x m³/mol	0.1	(Anon. 1988)
Mobility	Equilibrium distribution: air water solid	 *mass %* 0.05 1.50 98.44 (Anon. 1988).
Total degradation in water	100% of original compound found after 8 weeks in river water (initial concentration 0.010 mg/l) (Verschueren 1983). Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

EF

Bioconcentration factor, fishes	10–13 (Verschueren 1983) 2720–9060 10w,Cyprinus carpio, conc 0.00005 mg/l 2360–12600 10w, Cyprinus carpio, conc 0.000005 mg/l (lipid content 7.0%) 849–3250 10w, Cyprinus carpio, conc 0.00005 mg/l 1080–7450 10w, Cyprinus carpio, conc 0.000005 mg/l (lipid content 1.7%) (MITI 1992)
Bioconcentration factor, mollusca	500–2780 mussels (Verschueren 1983)
Other information about bioaccumulation	Confirmed to be accumulated on a high level (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	3 orl-rat 1.37 orl-mus 3 orl-mky (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	12 skn-rat (Lewis & Sweet 1984) 5–50 ukn-hmn (Virtanen & Nuuja 1987) 7.5–18 ukn-rat 29 ukn-mus (Virtanen & Nuuja 1987)
Other information about mammals	LD50, in food, short-tailed shrew (Blarina brevicauda), 87–174 mg/kg (Virtanen & Nuuja 1987). LDfr = 100 mg/kg/day, ALD 18 mg/kg, deer mouse (Peromyscus manicula-tus) (Virtanen & Nuuja 1987).
Health effects	0.2 mg/kg induces convulsions in human (Virtanen & Nuuja 1987).
LD50 values to birds in oral exposure, mg/kg	1.8 orl-brd 2 orl-bwd (Lewis & Sweet 1984) 2.37 orl-Agelaius phoeniceus 2.37–3.16 orl-Sturnus vulgaris 4.22 orl-Coturnix coturnix 1.78 orl-Passer domesticus 0.316–5.62 orl-Quiscalus quiscula 5.62 orl-Columba livia 1.5 orl-Falco sparverius 2.1 orl-Myiopsitta monachus (Schafer et al. 1983)
Effects on amphibia	LC50 0.0002 mg/l, 96hr, tadpoles of Rana hexadactyla (Khangarot et al. 1985).
Effects on arthropods	LC50 0.00025 mg/l, 96hr, Pteronarcys californica (Sanders & Cope 1968).
LC50 values to crustaceans, mg/l	0.039 48hr, Daphnia magna (Gorbach & Knanf 1971) 0.0009 120hr, Gammarus fasciatus (Sanders 1972) 0.9 act, Daphnia pulex (Frear & Boyd 1967) 368 48hr, Daphnia pulex (Priester 1966) 0.35 act, Daphnia magna (Kenaga 1979)
EC50 values to crustaceans, mg/l	20–352 48hr, Daphnia pulex (Shapiro 1979)

LC50 values to fishes, mg/l	0.0048	72hr, Stizostedion lucioperca
	0.00006	72hr, Coregonus
	0.00007	Poecilia reticulata
		72hr, Salmo gairdneri (Wohlgemuth 1977)
	0.00005	96hr, Menidia beryllina (Eisler 1970a)
	0.0006	96hr, Lepomis macrochirus (Henderson et al. 1959)
	0.0006	96hr, Salmo gairdneri (Katz 1961)
	0.001	48hr, Carassius auratus
	0.0008	48hr, Cyprinus carpio (Hashimoto & Nishiuchi 1981)
	0.0001	28d, 91.1%, Ictalurus melas
	0.034	96hr, Brachycentrus americanus (Anderson & Defoe 1980)
	0.59	96hr, Pimephales promelas (Priester 1966)
	0.0004	act, Lepomis macrochirus
	0.0086	act, Salmo gairdneri
	0.0011	act, Pimephales promelas (Kenaga 1979)
	2.9	48hr, Oryzias latipes (MITI 1992)
LOEC values to fishes, mg/l	0.0003	srv, chr, Cyprinodon variegatus (Ward & Parrish 1980)
	0.0003	srv, grw, chr, Cyprinodon variegatus (Hansen et al. 1977a)
	0.0003	rpd, chr, flag fish (Hermanutz 1978)
NOEC values to fishes, mg/l	0.0001	srv, grw, chr, Cyprinodon variegatus (Hansen et al. 1977a)
	0.0002	grw, chr, flag fish (Hermanutz 1978)
Other information	Impurity of dieldrin.	

986 • Epichlorohydrin

106-89-8

Synonyms	1-Chloro-2,3-epoxypropane ECH	
Sumformula of the chemical	C3H5OCl	
Use	In the manufacturing of epoxy resins, surface active agents, pharmaceuticals, insecticides and agricultural chemicals; solvent.	
State and appearance	Colourless liquid.	
Molecular weight	92.53	
Vapour pressure, mmHg	12	20 °C
	16.44	at 25 °C (Daubert & Danner 1985)
Water solubility, mg/l	60000	20 °C
	65000	20 °C
	65800	20 °C (Krijsheld & Vandergren 1986)
Melting point, °C	-57.2	(Howard I 1990)
	-57.2	(MITI 1992)
Boiling point, °C	116.5	760 mmHg, Howard I 1990
	116.1	760 mmHg (MITI 1992)

EF

Log octanol/water coefficient, log Pow	0.3	(Krijgsheld & Vandergren 1986)
Volatilization	Relative volatility (nBuAc=1) = 1.35 The half-life for evaporation of epichlorohydrin from a model river 1 m deep with a 1 m/sec current and 3 m/sec wind is 29hr, with the gas exchange rate playing a more dominant role than the liquid exchange rate. Epichlorohydrin is relatively volatile and would therefore readily evaporate from near-surface soils and other solid surfaces. (Lyman et al. 1980) (Howard I 1990)	
Photochemical degradation in air	Epichlorohydrin reacts with photochemically produced hydroxyl radicals with an estimated atmospheric half-life of 4 days. (Cupitt 1980) When irradiated in the presence of 5 ppm nitric oxide to simulate photochemical smog conditions, the half-life was 16hr. (Dilling et al. 1976)	
Hydrolysis in water	Epichlorohydrin hydrolyzes in distilled water to yield 1-chloro-2,3-propanediol (half-life 8.2 days at 20 °C). Acid catalysis contributes less than 10% to the rate of hydrolysis and base catalysis is not detectable at pH < 10. (Mabey & Mill 1978) In seawater epichlorhydrin will additionally react with chloride ions which will reduce its overall half-life to about 5.3 days, producing 1,3-dichloro-2-propanol as well as the hydrolysis product. (Santodonato 1980)	
Chemical oxygen demand, g 02/g	1.16	5 days (Brigie et al. 1979)
Biochemical oxygen demand, g 02/g	0.03	5 days (Bridie et al. 1979)
Total degradation in water	Biodegradation: 18% by BOD (hydrolyzed to 3-Chloro-propylene glycol) period: - substance: - sludge: - (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
Other information about degradation	In a laboratory biodegradability test using sewage seed, 3% of the theoretical BOD was consumed in 5 days. (Anderson 1983) With acclimated sewage seed, the percent of theoretical BOD consumed increased to 14%. (Bridie et al. 1979) Epichlorohydrin was confirmed to be significantly degraded in a laboratory test that utilizes an inoculum originating from soil, natural waters and sewage. (Sasaki 1978)	
Other information about bioaccumulation	Epichlorohydrin would not be expected to bioconcentrate appreciably in aquatic organisms. The log BCF has been estimated to be 0.66. (Santodonato 1980)	
LD50 values to mammals in oral exposure, mg/kg	90 40	orl-rat (Lewis & Sweet 1984) orl-rat (Verschueren 1983)
LD50 values to mammals in non-oral exposure, mg/kg	515	skn-rbt (Lewis & Sweet 1984)
TCLo values to mammals in inhalation exposure, ppm	20	ihl-hmn (Lewis & Sweet 1984)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 55 mg/l (Bringmann & Kühn 1980a)	
LOEC values to algae, mg/l	5.4	rpd, schr, Scenedesmus quadricauda (Bringmann & Kuhn 1980a)

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LC50 values to fishes, mg/l	24 48hr, Leuciscus idus 30.5 96hr, Branchydanio rerio (Wellens 1982) 23 24hr, Carassius auratus (Bridie et al. 1979) 35 96hr, Lepomis macrochirus 18 96hr, Menidia audens (Dawson et al. 1977)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 5.4 mg/l protozoa (Entosiphon sulcatum): 35 mg/l (Bringmann & Kühn 1980a)

987 • EPN

2104-64-5

Synonyms	O-Ethyl-O-4-nitrophenylphenylphosphonothioate Ethyl-p-nitrophenylbenzenethiophosphonate O-Ethyl-O-p-nitrophenyl-phenylthiophosphonate
Use	Insecticide, acaricide.
State and appearance	Light yellow crystals.
Molecular weight	323.32
Vapour pressure, mmHg	0.0003 100 °C
Water solubility, mg/l	0.91 (MITI 1992)
Melting point, °C	36 (MITI 1992)
Boiling point, °C	100 0.03 mmHg (MITI 1992)
Log octanol/water coefficient, log Pow	4.78 (MITI 1992)
Total degradation in water	Biodegradation: 3% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	659–1590 8w, Cyprinus carpio, conc 0.01 mg/l 358–1520 8w, Cyprinus crpio, conc 0.001 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be accumulated on a medium level (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	8 orl-rat 14.5 orl-mus 20 orl-dog (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	25 skn-rat 30 skn-rbt (Lewis & Sweet 1984)
Other information about mammals	LDfr = 37.5 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

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LD50 values to birds in oral exposure, mg/kg	3	orl-dck
	5	orl-qal (Lewis & Sweet 1984)
	3.16	orl-Agelaius phoeniceus
	7.5	orl-Sturnus vulgaris
	10	orl-Coturnix coturnix
	2.37	orl-Passer domesticus
	4.22	orl-Quiscalus quiscula
	4.22	orl-Columba livia
	5.62	orl-Molothrus ater (Schafer et al. 1983)
LC50 values to crustaceans, mg/l	0.0012	Daphnia pulex (Nishiuchi & Hashimoto 1969)
	0.00056	96hr, Palaemonetes kadiakensis
	0.007	96hr, Gammarus fasciatus (Sanders 1972)
	0.0034	96hr, Mysidopsis bahia (Anon. 1981)
	0.00029	96hr, Penaeus duorarum (EPA 600/4-81-041)
LC50 values to fishes, mg/l	0.21	act, Salmo gairdneri
	0.37	act, Lepomis macrochirus (Pesticide Manual 1983)
	0.19	96hr, Cyprinodon variegatus
	0.018	96hr, Lagodon rhomboides (Anon. 1981) (EPA 600/4-81-041)
	0.35	48hr, Cyprinus carpio (Nishiuchi & Hashimoto 1967)
	0.1	96hr, Lepomis macrochirus (Sanders & Cope 1968)
	10.6	48hr, Oryzias latipes (MITI 1992)

988 • 9,10-Epoxystearic acid 2443-39-2

LC50 values to fishes, mg/l	1.5	96hr, Salmo gairdneri (Leach & Thakore 1975)

989 • EPTC 759-94-4

Synonyms	S-Ethyl dipropylthiocarbamate S-Ethyl-N,N-dipropyl(thiocarbamate) Ethyl N, N-di-N-propylthiocarbamate	
Use	Active ingredient in selective herbicides.	
Way to effect	Selective.	
Molecular weight	189.35	
Vapour pressure, mmHg	0.035	25 °C
Water solubility, mg/l	370	
Log soil sorption coefficient, log Kom	2.38	(Sabljic 1987)
Half-life in soil, days	30	(Li et al. 1990)
Total degradation in soil	75–100% disappearance from soils: 4 weeks (Verschueren 1983).	

LD50 values to mammals in oral exposure, mg/kg	1325 orl-rat 750 orl-mus 112 orl-cat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	1460 skn-rbt (Lewis & Sweet 1984)
LCLo values to mammals in inhalation exposure, mg/kg	200 4hr, ihl-rat (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	100 orl-bwd (Lewis & Sweet 1984) 100 orl-Agelaius phoeniceus > 100 orl-Sturnus vulgaris (Schafer et al. 1983)
Effects on plants	Winter wheat (Tritium sativum) was grown 21 days in sand which contained 0.25 mg EPTC per kg air day sand → root fresh weight was decreased by 19% and phospholipid fatty acid content by 51 %. Karunen & Wilkinson 1975. – Tubers of Cyperus rotundus L. were planted to soil sprayed with 0.25 kg EPTC/ha → a decrease in number of sprouts above ground (3 weeks after treatment). Rincon & Warren 1979. – Wheat (Triticum aestivum) was grown for 14 days in complete mineral solution containing EPTC.Gibberellic acid (GA) content was decreased 96% by 125 ppbw ETCP.Wilkinson et al. 1981. – Incubation of segments of barley coleoptile and Sesbania exaltata hypocotyls in 1% sucrose containing 2 ppm EPTC inhibited protein synthesis by 38 and 14%, respectively (Mann et al. 1965). – Germinated seedlings of barley (Hordeum vulgare) were grown in EPTC-treated silica sand: 18 ppm EPTC (in mg active material per litre solution;12 ml of the solution was added to 225 g dry sand) caused 50% root inhibition over 72hr. (O'Sullivan & Prendeville 1974)
LC50 values to crustaceans, mg/l	0.63 act, Daphnia magna (Kenaga 1979)
LC50 values to fishes, mg/l	19 96hr, Salmo gairdneri 27 96hr, Lepomis macrochirus (Anon. 1973b) 27 act, Lepomis macrochirus 19 act, Salmo gairdneri > 20 act, Pimephales promelas (Kenaga 1979)

990 • Essolvene 37226-28-1

Effects on the physiology of water organisms	Cyprinus carpio; 15.2 mg/l, 0.01d, biochemical effect (change in physiochemical process including glycogen uptake, cholesterol levels and lipid analysis) (Nakanishi et al. 1986).
Other information about water organisms	Cyprinus carpio; 15.2 mg/l; 0.01d, 100% mortality or 0% surviving including algicidal and herbicidal effects (Nakanishi et al. 1986).

991 • Ethanediol ester montanic acid 26787-65-5

Sumformula of the chemical	C30H6003	
Water solubility, mg/l	< 10	(MITI 1992)
Melting point, °C	80–82	(MITI 1992)
Log octanol/water coefficient, log Pow	5.1	(MITI 1992)

Total degradation in water	Biodegradation: 8–28% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 1.3–12 6w, Cyprinus carpio, conc 1 mg/l < 12–29 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	260 48hr, Oryzias latipes (MITI 1992)

992 • Ethanol 64-17-5

Synonyms	Methylcarbinol Ethylalcohol	
Sumformula of the chemical	C2H6O	
Use	Solvent.	
Molecular weight	46.07	
Melting point, °C	-117.3	
Boiling point, °C	78.5	
Log octanol/water coefficient, log Pow	-0.3	(Sangster 1989)
Henry's law constant, Pa x m³/mol	0.8234 0.6373	calc. (Yaws et al. 1991) (Hine & Mookerjee 1975)
Volatilization	Relative volatility (nBuAc=1) = 3.3	
LD50 values to mammals in oral exposure, mg/kg	21000	orl-rat
Maximum longterm immission concentration in air for plants, mg/m³	100	VDI 2306
Maximum longterm immission concentration in air for plants, ppm	50	VDI 2306
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 6500 mg/l (Bringmann & Kühn 1980a)	
EC50 values to microorganism, mg/l	33672	Biodegradation inhibition (Vaishnav 1986)
LC50 values to crustaceans, mg/l	9268–14221	48hr, Daphnia magna (Takahashi et al. 1987)
	3715–6772	48hr, Daphnia magna (Takahashi et al. 1987)
	7750	96hr, 10 °C, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	11200	24hr, Salmo trutta (Majewski et al.1978)
	11050	7d, Poecilia reticulata (Smith 1974)
	14200	96hr, Pimephales promelas (Veith et al. 1983)
	10000–11500	96hr, 10 °C (Linden et al. 1979)

Other information about water organisms	LOEC 65 mg/l, rpd, schr, Entosiphon sulcatum (Bringmann & Kühn 1980a). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 5000 mg/l protozoa (Entosiphon sulcatum): 65 mg/l (Bringmann & Kühn 1980a).

993 • Ethion

563-12-2

Synonyms	0,0,0',0'-Tetraethyl-S,S'-methylenedi-(phosphorodithioate)
Use	Insecticide, acaricide.
Molecular weight	384.49
Vapour pressure, mmHg	0.0000015 25 °C
Melting point, °C	-12– -15
Log soil sorption coefficient, log Kom	4.19 (Sabljic 1987)
Total degradation in water	50% of original compound found after 8 weeks in river water (initial concentration 10 µg/l) (Verschueren 1983).
LD50 values to mammals in oral exposure, mg/kg	13 orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	62 skn-rat (Lewis & Sweet 1984)
TDLo values to mammals in oral exposure, mg/kg	0.1 orl-hmn (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	45 orl-bwd (Lewis & Sweet 1984) 45.0–58.0 orl-Agelaius phoeniceus 304 orl-Sturnus vulgaris (Schafer et al. 1983)
LC50 values to crustaceans, mg/l	0.00001 act, Daphnia magna (Kenaga 1979) 0.005 act, Daphnia pulex (Nishiuchi & Hashimoto 1967) 0.0018 96hr, Gammarus lacustris (Sanders 1969)
LC50 values to fishes, mg/l	0.23 act, Salmo gairdneri (Kenaga 1979) 0.15 96hr, Micropterus salmoides (Verschueren 1983) 0.56 96hr, Salmo gairdneri (Verschueren 1983) 1.2 48hr, Cyprinus carpio (Nishiuchi & Hashimoto 1967)

994 • Ethofumesate

26225-79-6

Use	Active ingredient in herbicides.
Effects on plants	Ethofumesate reduced germination of dodder (Cuscuta australis) seeds by 82% and reduction of stem elongation was 25% at a concentration of 10 µg/ml (seeds/seeds with shoots were placed to Petri dishes on filter paper where the herbicide solution was added). There was a decrease in seedling emergence and height of dodder sown in a silt loam soil treated with 0.8 kg ethofumesate /ha (Giannopolitis 1979).
LC50 values to fishes, mg/l	15 24hr, Poecilia reticulata (Pesticide Manual 1983)

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995 • Ethoprop 13194-48-4

Synonyms	O-Ethyl-S,S-dipropylphosphorodithioate Mocap Prophos ENT 27318	
Molecular weight	242.36	
LD50 values to mammals in oral exposure, mg/kg	34	orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	26	skn-rbt (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	1.26 5.5 4.22 7.5 7.5 4.21 10 13.3	orl-dck orl-ckn (Lewis & Sweet 1984) orl-Agelaius phoeniceus orl-Sturnus vulgaris orl-Coturnix coturnix orl-Passer domesticus orl-Quiscalus quiscula orl-Columba livia (Schafer et al. 1983)
LD50 values to birds in dermal exposure, mg/kg	11	skn-dck (Lewis & Sweet 1984)
LC50 values to crustaceans, mg/l	0.0075 0.013	96hr, Mysidopsis bahia (Anon. 1981) (EPA 600/4-81-041) 96hr, Penaeus duorarum (Pesticide Manual 1983)
LC50 values to fishes, mg/l	0.0063 0.18	96hr, Lagodon rhomboides 96hr, Cyprinodon variegatus (Pesticide Manual 1983)

996 • 4-Ethoxyaniline 156-43-4

Melting point, °C	4.5	(MITI 1992)
Boiling point, °C	254.2–254.7	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance. 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).	
Bioconcentration factor, fishes	< 1 < 10	6w, Cyprinus carpio, conc 1 mg/l 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/	100	48hr, Oryzias latipes (MITI 1992)

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997 • Ethyl acetate

141-78-6

Synonyms	Acetic acid ethyl ester Acetic ether Ethylacetic ester Ethyl ethanoate Vinegar naphtha Acetidin
Sumformula of the chemical	C4H8O2
Purity, %	85–88% 95–98%
Known impurities	Oponite ethanate, 0.00125%; Methyl isobutyl ketone, 0.01%, Ethanol, 0.05%.
Use	Solvent. Synthetic flavouring; adjuvant.
State and appearance	Colourless liquid. Will float in slick and dissolve at moderate rate.
Odour	Pleasant, fruity odour. Recognition odour 50 ppm in air. Quality: sweet, ester Hedonic tone: pleasant Threshold odour concentration absolute: 6.3 ppm 50% recognition: 13.2 ppm 100% recognition: 13.2 ppm Odour index 100% recognition: 7 575 (Hellman & Small 1974).
Molecular weight	88.1
Specific gravity (water=1)	0.9
Vapour density (air=1)	3.04
Vapour pressure, mmHg	76 20 °C 69 19 °C (Ambrose 1981)
Water solubility, mg/l	87000 20 °C 64000 (Wasik 1981)
Melting point, °C	-83.6
Boiling point, °C	77
Log octanol/water coefficient, log Pow	0.73 (Hansch & Leo 1979) 0.73 (Sangster 1989)
Henry's law constant, Pa x m³/mol	12.2 (Bocek 1976)
Volatilization	Relative volatility (nBuAc=1) = 4.2
Mobility	Ethyl acetate is very soluble in water and therefore would not be expected to adsorb significantly to soil (Lyman et al. 1960).
Photochemical degradation in air	Ethyl acetate reacts with photochemically produced hydroxyl radicals in the atmosphere by H-atom abstraction from the OCH2 entity with a measured half-life of 8.3 days (12hr sunlit day, clean atmosphere) and 2.1 days (12hr sunlit day, moderately polluted atmosphere) (Campbell 1978).
Hydrolysis in water	Slowly hydrolyses to acetic acid ethanol. Ethyl acetate is resistant to hydrolysis under neutral conditions. The base catalyzed process is dominant and leads to a half-life of 2 yr at pH 7 and 25 °C (Mabey & Mill 1978).

Other information about degradation	Biodegrades at moderate rate (Sax 1986). Ethyl acetate is normally easily biodegraded. Reported 5 day BOD values using a sewage inoculum range from 36 to 68% of theoretical with the value being somewhat reduced in salt water (Howard 1990).
Other information about bioaccumulation	Potential for accumulation: negative (Sax 1986).
LD50 values to mammals in oral exposure, mg/kg	11300 orl-rat 4935 orl-rbt (Sax 1986) 5500 orl-gpg 4100 orl-mus 5620 orl-rat (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	709 ipr-mus 3000 scu-cat, scu-gpg (Sax 1986)
LC50 values to mammals in inhalation exposure, ppm	1600 ihl-rat (Sax 1986)
LDLo values to mammals in non-oral exposure, mg/kg	5000 scu-rat (Sax 1986)
LCLo values to mammals in inhalation exposure, mg/kg	31000 103min, ihl-mus 61000 ihl-cat 77 60min, ihl-gpg (Sax 1986)
TDLo values to mammals in non-oral exposure, mg/kg	3600 ipr-mus, tumorigenic (Sax 1986)
TCLo values to mammals in inhalation exposure, ppm	400 ihl-hmn (Sax 1986)
Other information about mammals	Skin and eye irritation: eye, human, 400 ppm (Sweet 1987).
Health effects	Direct contact: Moderately irritating eyes, mucous membranes, gums, and respiratory tract. Anesthetic over 2000 ppm. Prolonged inhalation can cause renal or hepatic damage. Prolonged contact can cause conjunctival irritation and corneal clouding (Sax 1986). Moderately toxic via all routes with acute exposure. Toxic chronically to a lesser degree via all routes. Irritant (Sax 1986). Skin and eye irritation: eye-hmn 400 ppm (Sax 1986).
Carcinogenicity	Rat-tumor, negative – in diet 300 days (Sax 1986).
Mutagenicity	Mutation data: cyt, ham, fbr, 9000 mg/l; sin, smc, 24400 ppm (Sweet 1987).
Maximum longterm immission concentration in air for plants, mg/m³	75 VDI 2306
Maximum longterm immission concentration in air for plants, ppm	20 VDI 2306
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 650 mg/l (Bringmann & Kühn 1980a).
Effects on wastewater treatment	1000 mg/l was not substrate limiting to anaerobic processes (Sax 1986).

LOEC values to algae, mg/l	15	rpd, schr, Scenedesmus quadricauda (Bringmann & Kuhn 1980a)
NOEC values to algae, mg/l	2000	rpd, schr, Selenastrum capricornutum (Slooff et al. 1983)
LC50 values to crustaceans, mg/l	720 260 160 1600 750	48hr, Daphnia magna (Canton & Adema 1978) 48hr, Daphnia pulex (Canton & Adema 1978) 48hr, Daphnia cucullata (Canton & Adema 1978) 48hr, Asellus aquaticus (Slooff 1983) 48hr, Gammarus pulex (Slooff 1983)
LC50 values to fishes, mg/l	125	48hr, Ozyrias latipes (Slooff et al. 1983)
Other information about water organisms	LC50, 48hr, 760 mg/l, Tubificidae LC50, 48hr, 750 mg/l, Chironomus gr. thummi LC50, 48hr, 1200 mg/l, Erpobdella octoculata LC50, 48hr, 1100 mg/l, Lymnaea stagnalis LC50, 48hr, 3020 mg/l, Dugesia cf. lugubris LC50, 48hr, 1350 mg/l, Hydra oligactis LC50, 48hr, 600 mg/l, Corixa punctata LC50, 48hr, 600 mg/l, Ischura elegans LC50, 48hr, 130 mg/l, Nemoura cinerea LC50, 48hr, 480 mg/l, Cloeon dipterum (Slooff 1983). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 15 mg/l protozoa (Entosiphon sulcatum): 202 mg/l (Bringmann & Kühn 1980a).	
Other information	Air pollution: low (Sax 1986).	

998 • Ethyl acrylate

140-88-5

Synonyms	Propenoic acid, ethyl ester	
Sumformula of the chemical	C5H8O2	
Use	Solvent.	
Odour	Quality: sour, pungent Hedonic tone: unpleasant Threshold odour concentration absolute: 0.0002 ppm 50% recognition: 0.00030 ppm 100% recognition: 0.00036 ppm Odour index 100% recognition: 113 000 000 (Hellman & Small 1974).	
Water solubility, mg/l	15000 15000	20 °C (MITI 1992)
Boiling point, °C	99.4 99.7	 (MITI 1992)
Log octanol/water coefficient, log Pow	1.32	(Sangster 1989)
Volatilization	Relative volatility (nBuAc=1) = 3.3	
Total degradation in water	Biodegradation: 52% by BOD (on the upward trend) period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

EF

Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	1000 orl-rat

999 • 2-Ethyl anthraquinone 84-51-5

Melting point, °C	108.2–110.4 (MITI 1992)
Log octanol/water coefficient, log Pow	3.91 Anon. 1986 4.05 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).
Bioconcentration factor, fishes	7.8–12.4 8w, Cyprinus carpio, conc 0.135 5.6–13.5 8w, Cyprinus carpio, conc 0.135 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be accumulated on a medium level (Anon. 1987).
LC50 values to fishes, mg/l	13.5 48hr, Oryzias latipes (MITI 1992)

1000 • Ethyl benzoate 93-89-0

Synonyms	Benzoic acid, ethyl ester
Sumformula of the chemical	C9H10O2
Use	Flavoring, perfumery, solvent mixture, lacquers, solvent for many cellulose derivatives and natural and synthetic resins.
State and appearance	Colourless aromatic liquid.
Specific gravity (water=1)	1.043–1.046
Boiling point, °C	212.9
Flashing point, °C	93
Log octanol/water coefficient, log Pow	2.64 (Anon. 1986) 2.64 (Sangster 1989)
Other physicochemical properties	Soluble in alcohol and ether, insoluble in water. Combustible.

1001 • Ethyl ether 60-29-7

Synonyms	Diethyl ether Anesthetic ether Diethyl oxide Ether Ethoxyethane 1,1'-Oxybisethane
Sumformula of the chemical	C4H10O
Use	Solvent.

EF

Molecular weight	74.14
Water solubility, mg/l	69000 20 °C > 1000 (MITI 1992)
Melting point, °C	-116.2 (MITI 1992)
Boiling point, °C	34.5 (MITI 1992)
Log octanol/water coefficient, log Pow	0.8 (Anon. 1986) 0.89 (Sangster 1989)
Volatilization	Relative volatility (nBuAc=1) = 11
Total degradation in water	Biodegradation: 2.5% by TOC period: 28d substance: 100 mg/l sludge: 30 mg/l 6.5% by GC analysis period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	0.9–1.4 6w, Cyprinus carpio, conc 0.5 mg/l < 1.7–9.1 6w, Cyprinus carpio, conc 0.050 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	1215 orl-rat (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	2000 ipr-gpg 2420 ipr-mus 996 ivn-mus (Sweet 1987)
LDLo values to mammals in oral exposure, mg/kg	420 orl-hmn 260 orl-man (Sweet 1987)
LDLo values to mammals in non-oral exposure, mg/kg	8 scu-mus (Sweet 1987)
LCLo values to mammals in inhalation exposure, ppm	76000 ihl-dog ihl-rbt (Sweet 1987) 106000 ihl-dog ihl-rbt (Sweet 1987)
TCLo values to mammals in inhalation exposure, ppm	200 ihl-hmn (Sweet 1987)
Effects on amphibia	Frog, subcutaneous, LDLo 24 mg/kg (Sweet 1987).
EC50 values to microorganism, mg/l	5600 15 min Microtox (Hermens et al. 1985)
LC50 values to fishes, mg/l	> 10000 96hr, Lepomis macrochirus > 10000 96hr, Menidia audens (Dawson et al. 1977) 2138 14d, Poecilia reticulata (Könemann 1979) > 1000 48hr, Oryzias latipes (MITI 1992)

1002 • Ethyl isodehydroacetate 3385-34-0

Other information about mammals	ALD = 100.0 mg/kg, act , orl, deer mouse (Virtanen & Nuuja 1987).

1003 • Ethyl phenyl ether 103-73-1

Synonyms	Phenetole
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

1004 • Ethyl salicylate 118-61-6

LC50 values to fishes, mg/l	19.6 14.9	96hr, Pimephales promelas 96hr, Ictalurus punctatus (Holcombe et al. 1984)
Other information about water organisms	LC50, > 25.9 mg/l, 96hr, snail (Holcombe et al. 1984)	

E

1005 • N-Ethyl-1-aminonaphthalene 118-44-5

Synonyms	1-Naphthalenamine, N-ethyl-	
Sumformula of the chemical	C12H13N	
EINECS-number	2042503	
Water solubility, mg/l	110	(MITI 1992)
Log octanol/water coefficient, log Pow	3.45	(MITI 1992)
Total degradation in water	Biodegradation: 0–8% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	120–251 127–292	8w, Cyprinus carpio, conc 0.1 mg/l 8w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	7.4	48hr, Oryzias latipes (MITI 1992)

1006 • 2-Ethyl-1-hexanol hydrogen phosphate 298-07-7

Synonyms	HDEHP Bis(2-ethylhexyl)hydrogen phosphate Di(2-ethylhexyl)phosphoric acid	
Sumformula of the chemical	C16H35O4P	
Water solubility, mg/l	182	(MITI 1992)

Melting point, °C	< -60 (MITI 1992)
Log octanol/water coefficient, log Pow	2.67 (MITI 1992)
Total degradation in water	Biodegradation: 0–17% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	1.1–2.4 6w, Cyprinus carpio, conc 1 mg/l 2.7–6.0 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	48–54 96hr, Salmo gairdneri (Dave & Lindman 1978) 148 48hr, Oryzias latipes (MITI 1992)

1007 • 2-Ethyl-2-hexenal 645-62-5

Sumformula of the chemical	C8H14O
Water solubility, mg/l	586 (MITI 1992)
Boiling point, °C	195 (MITI 1992)
Total degradation in water	Biodegradation: 79.0–99.9% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

1008 • Ethyl-4-aminobenzoate 94-09-7

Synonyms	Ethyl-p-aminobenzoate Benzocaine
Use	Medicine; suntan preparations.
State and appearance	White, crystalline, odourless, tasteless powder.
Odour	Odourless.
Molecular weight	165.19
Melting point, °C	88–90 °C
Other information about degradation	Impact on biodegradation: NH3 oxidation by Nitrosomonas sp.: at 100 mg/l: 30% inhibition at 50 mg/l: 27% inhibition at 10 mg/l: 0% inhibition (Verschueren 1983).
LD50 values to birds in oral exposure, mg/kg	56 orl-Agelaius phoeniceus 316 orl-Sturnus vulgaris (Schafer et al. 1983)
LC50 values to fishes, mg/l	35 96hr, Pimephales promelas (Holcombe et al. 1984)

1009 • Ethyl-N-phenylcarbamate

101-99-5

Synonyms	Ethyl phenylcarbamate Ethyl phenylurethane
Sumformula of the chemical	C9H11NO2
State and appearance	White, crystalline solid.
Odour	Aromatic odour; clove-like taste.
Melting point, °C	51
Log soil sorption coefficient, log Kom	1.58 (Sabljic 1987)
Other physicochemical properties	Soluble in alcohol, ether and boiling water; insoluble in cold water.
LD50 values to birds in oral exposure, mg/kg	> 100 orl-Agelaius phoeniceus > 100 orl-Sturnus vulgaris (Schafer et al. 1983)

1010 • N-Ethyl-p-toluidine

622-57-1

Water solubility, mg/l	1000 (MITI 1992)
Boiling point, °C	217 (MITI 1992)
Log octanol/water coefficient, log Pow	2.32 (MITI 1992)
Total degradation in water	Biodegradation: 2% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.2–4.1 6w, Ctprinus carpio, conc 0.2 mg/l < 2.2 6w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	62.5 48hr, Oryzias latipes (MITI 1992)

1011 • Ethylaceto acetate

141-97-9

Synonyms	Diacetic ester Ethyloacetoate Acetoacetic ester Butanoic acid, 3-oxo, ethyl ester Acetoacetic acid ethyl ester
Sumformula of the chemical	C6H10O3
Purity, %	> 99%
Known impurities	Major impurities: ethyl acetate, ethanol, acetone.
Use	Intermediate in the manufacture of dyes, pesticides and pharmaceuticals.
Water solubility, mg/l	116000 at 20 °C
Melting point, °C	-40

Boiling point, °C	180	at 1013 hPa
Flashing point, °C	71	PENSKY-MARTENS CLOSED CUP
Log octanol/water coefficient, log Pow	-0.162	at 25 °C, measured, EG-Richtlinie AB OECD Guideline 107, Wacker-Chemie GmbH
Half-life in air, days	10.33	at 25 °C,
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 33 mg/l (Bringmann & Kühn 1980a).	
LOEC values to algae, mg/l	7.6	rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 7.6 mg/l protozoa (Entosiphon sulcatum): 391 mg/l (Bringmann & Kühn 1980a)	

1012 • Ethylamine 75-04-7

Synonyms	Aminoethane	
Sumformula of the chemical	C2H7N	
pKa	10.7	
Log octanol/water coefficient, log Pow	-0.13	(Sangster 1989)
LD50 values to birds in oral exposure, mg/kg	> 101	orl-Agelaius phoeniceus (Schafer et al. 1983)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 29 mg/l (Bringmann & Kühn 1980a).	
LOEC values to algae, mg/l	1.3 2.3	rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976) rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 2.3 mg/l protozoa (Entosiphon sulcatum): 45 mg/l (Bringmann & Kühn 1980a).	

1013 • Ethylamine hydrochloride 557-66-4

Sumformula of the chemical	C2H8NCl	
Water solubility, mg/l	> 100000	(MITI 1992)
Melting point, °C	113.3	(MITI 1992)
Total degradation in water	Biodegradation: 57–60% by BOD (on the upward trend) period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

1014 • N-Ethylaniline 103-69-5

Sumformula of the chemical	C8H11N	
Melting point, °C	-63.5	(MITI 1992)
Boiling point, °C	206	(MITI 1992)

pKa	5.12	(Sangster 1989)
Log octanol/water coefficient, log Pow	2.16	(Sangster 1989)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).	
Bioconcentration factor, fishes	3–11 < 6–13	6w, Cyprinus carpio, conc 1 mg/l 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	105	48hr, Oryzias latipes (MITI 1992)

1015 • Ethylbenzene 100-41-4

Sumformula of the chemical	C8H10	
Use	Intermediate; petrol additive.	
Molecular weight	106	
Water solubility, mg/l	177 131 161 180	25 °C (Polak & Lu 1973) 25 °C (Price 1976) 25 °C (Sutton & Calder 1975) (MITI 1992)
Melting point, °C	-94.97 -94.95	(Suntio et al. 1988) (MITI 1992)
Boiling point, °C	152.4 136.186	 (MITI 1992)
Log octanol/water coefficient, log Pow	3.15 3.13 3.13 3.15 3.26 3.13 3.12 3.12 3.15	(Anon. 1986) (Chin et al. 1986) (Anon. 1988) (Hansch & Leo 1979) (Hammers et al. 1982) (Miller et al. 1984) (Hanai et al. 1981) (D'Amboise & Hanai 1982) (Sangster 1989)
Henry's law constant, Pa x m^3/mol	729.9 864 815	calc. (Suntio et al. 1988) exptl. (Suntio et al. 1988) calc. (Yaws et al. 1991)
Mobility	Equilibrium distribution: air water solid	 *mass %* 99.35 0.54 0.11 (Anon. 1988).

Total degradation in water	Biodegradation: 81–126% by BOD period: 14d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).
LD50 values to mammals in oral exposure, mg/kg	3800 orl-rat
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 12 mg/l (Bringmann & Kühn 1980a).
LOEC values to algae, mg/l	33 rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to crustaceans, mg/l	75 48hr, Daphnia magna (LeBlanc 1980)
LC50 values to fishes, mg/l	42.3 96hr, Pimephales promelas 32 96hr, Lepomis macrochirus (Pickering & Henderson 1966) 150 96hr, Lepomis macrochirus (Buccafusco et al. 1981) 280 96hr, Cyprinodon variegatus (Heitmuller et al. 1981)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): > 160 mg/l protozoa (Entosiphon sulcatum): 140 mg/l (Bringmann & Kühn 1980a)

1016 • Ethylbutyrate 105-54-4

Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 140 mg/l (Bringmann & Kühn 1980a).
LOEC values to algae, mg/l	47 rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 47 mg/l protozoa (Entosiphon sulcatum): 236 mg/l (Bringmann & Kühn 1980a).

1017 • Ethylchlorocarbonate 541-41-3

Synonyms	Ethyl chloroformate
Use	Organic synthesis, intermediate in making diethyl carbonate, flotation agents, polymers, isocyanates.
State and appearance	Water-white liquid.
Odour	Irritating odour.
Melting point, °C	< -10 (MITI 1992)
Boiling point, °C	94–95 (MITI 1992)
Flashing point, °C	16.1 closed cup
Other physicochemical properties	Decomposes in water and alcohol; soluble in benzene, chloroform, and ether. Flammable, dangerous fire risk. Strong irritant to eyes and skin.

Total degradation in water	Biodegradation: 81–86% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

1018 • Ethylene

74-85-1

Synonyms	Ethene
Odour	Quality: olefinic Hedonic tone: unpleasant to neutral Threshold odour concentration absolute: 260 ppm 50% recognition: 400 ppm 100% recognition: 700 ppm Odour index 100% recognition: 1 428 (Hellman & Small 1974).
Molecular weight	28.05
Melting point, °C	-169
Boiling point, °C	-103.7
Henry's law constant, Pa x m^3/mol	21030 calc. (Yaws et al. 1991)
Effects on plants	0.002–0.02 ppm (0.0023–0.023 mg/m^3) for 24 (nonwoody plants susceptible to ethylene) (U.S. Environmental Protection Agency 1976).

1019 • Ethylene imine

151-56-4

Use	Solvent.
Boiling point, °C	56–57
LD50 values to mammals in oral exposure, mg/kg	15 orl-rat
Carcinogenicity	Carcinogen (Anon. 1974).
Mutagenicity	Mutagen (Verschueren 1983).
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 5.5 mg/l (Bringmann & Kühn 1980a)
LOEC values to algae, mg/l	0.12 srv, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 0.37 mg/l protozoa (Entosiphon sulcatum): 4.3 mg/l (Bringmann & Kühn 1980a)

1020 • Ethylene oxide

75-21-8

Synonyms	1,2-Epoxyethane Dihydrooxirene Dimethyleneoxide Ethene oxide Oxane α, β-Oxidoethane Oxirane
Sumformula of the chemical	C2H4O
Products containing the chemical	* Pure products: Anprolene Melgas Merpal Sterigas P * Formulations with carbon dioxide: Carboxide Cartox Etox Oxyfume 20 Oxyfume 30 Sterigas 90/10 Steroxide 20 T-gas * Formulations with fluorocarbons: Oxyfume 12 Sterigas 12/88 Steroxide 12/88 Etoxiat
Purity, %	100
Use	Intermediate in the production of various chemicals: the antifreeze 1,2-ethanediol; polyethylene terephthalate polyesters for fibres, films, and bottles; non-ionic surface active agents; glycol ethers; ethanolamines; and choline. A small fraction of the total consumption was used as an antimicrobial sterilant or as an insecticidal fumigant (WHO 1978, Glaser 1979). Less than 0.02% of this production was used for sterilization in hospitals (Glaser 1979). In Belgium small fraction was also used in the health care and medical products industries (Wolfs et al. 1983).
State and appearance	Colourless solution or gas.
Odour	Ethereal (Jacobson et al.1956, Hellman & Small 1974) Odour threshold for perception: 470 mg/m³ Odour threshold for recognition: 900–1260 mg/m³. Recognition level 1.5 mg/m³ in air (Sax 1986). Quality: sweet, olefinic Hedonic tone: neutral Threshold odour concetration absolute: 260 ppm 50% recognition: 500 ppm 100% recognition: 500 ppm Odour index 100% recognition: 2 000 (Hellman & Small 1974)
Molecular weight	44.06
Specific gravity (water=1)	0.882
Vapour density (air=1)	1.52

Density, kg/m^3	870	20 °C
Conversion factor, 1 ppm in air=	1.8	mg/m^3 at 25 °C
Vapour pressure, mmHg	1095 200	20 °C -19.5 °C
Melting point, °C	-111	
Boiling point, °C	10.4	
Flashing point, °C	-18	
Log octanol/water coefficient, log Pow	-0.3	(Sangster 1989)
Volatilization	Evaporation from water is a significant removal process. Under specific concentrations, a half-life of 1hr was found for the evaporation of ethylene oxide from water (WHO 1985).	
Mobility	The main pathway of entry of ethylene oxide into the environment is through its escape into the atmosphere due to evaporation and with vented gases during production, handling, storage, transport, and use. Most of the ethyleneoxide applied as a sterilant or fumigant will enter the atmosphere (Bogyo et al. 1980).	
Other physicochemical properties	Very flammable, combustion imminent. Toxic combustion products: hazardous. Explosiveness: Reactive under confinement, extreme caution. Vapour forms explosive mixtures with air over wide range. May rearrange chemically and/or polymerize violently with evolution of heat in contact with catalytic surfaces. Miscible, 25 °C.	
Other reactions in atmosphere	At ambient levels, ethylene oxide will be removed from the atmosphere via oxidation by hydroxyl radicals. On the basis of a theoretical rate constant for this reaction, the atmospheric residence time of ethylene oxide was estimated to be 5.8 days (Cupitt 1980). However, experimental data have shown the residence time to be 100–215 days, depending on the hydroxyl radical concentration and the ambient temperature (US EPA 1985). Because of its high water solubility, ethylene oxide levels in air will also be reduced through washout by rain (Conway et al.1982). The photochemical reactivity of ethylene oxide, in terms of its ozone forming ability, is low (Joshi et al.1982).	
Hydrolysis in water	Hydrolysis to 1,2-ethanediol results in detoxification. The toxicity of 2-chloroethanol for aquatic organisms resembles that of ethylene oxide, though 2-chloroethanol seems to be more toxic for Daphnia magna . Nevertheless, under environmental conditions, the conversion of ethylene oxide to 2-chloroethanol or 1,2-ethanediol will be slow (WHO 1985).	
Chemical oxygen demand, g 02/g	1.74	5 days (Bridie et al. 1979)
Other chemical degradation processes	In the environment, chemical degradation in water through ionic reactions appears to be comparativily slow. In neutral, fresh water at 25 °C, ethylene oxide is broken down to form 1,2-ethanediol with a half-life of 14 days (Conway et al.1983). At 0 °C, the half-life is 309 days. The reaction is acid-base-catalysed (Virtanen 1963). In the presence of halide ions, 2-haloethanol will also be formed. In neutral water of 3% salinity, at 25 °C, 77% of ethylene oxide was found to react to form 1,2-ethanediol and 23%, to form 2-chloroethanol with a half-life of 9 days (Conway et al.1983).	
Biochemical oxygen demand, g 02/g	0.06	5 days (Bridie et al. 1979)
Aerobic degradation in water	Ethylene oxide and its possible metabolites can be biodegraded slowly by aerobic microorganisms. Biological oxygen demands of 3–5% and 52% of the theoretical oxygen demand were determined for ethylene oxide after 5 and 20 days, respectivily, using a domestic sewage seed (Bridie et al.1979b; Conway et al.1983).	

Metabolism in mammals	In dogs, peak levels of 13 and 33 mg 1,2-ethanediol /litre blood-plasma were measured between 1 and 3hr after intravenous administration of 25 or 75 mg ethylene oxide in water /kg body weight, respectively . As the half-life for hydrolysis is about 60hr at 40 °C in neutral fresh water (Virtanen 1963) the involvement of an epoxide-hydrolase has been suggested, but this has not yet been confirmed. The peak concentration of 1,2-ethanediol at 25 mg ethylene oxide /kg body weight represented approximately 25% of the dose of ethylene oxide. Within 24hr, 7–24% of the dose was excreted in the urine as 1,2-ethanediol. No other compound-related metabolites were identified (Martis et al.1982). The results of studies on rats, rabbits, and monkeys have shown that some 1,2-ethanediol is metabolized but that most of it is excreted unchanged in the urine (Gessner et al.1961; McChessney et al.1971). When a single dose of 2 mg labelled ethylene oxide in propanediol /kg body weight was applied intraperitoneally to rats, 43 % of the administered radioactivity was excreted in the urine within 50hr (41 % within 24hr) of exposure, 9 % as S-(2-hydroxyethyl)cysteine and 33 % as N-acetyl-S-(2-hydroxyethyl)cysteine, both products of glutathione-conjugation. Via the lungs, 1.5 % was excreted as $CO2$ and 1 % as unmetabolized ethyleneoxide (Jones & Wells 1981). The involvement of glutathione-epoxide-S-transferase has not been investigated further. In vitro glutathione-conjugation of the homologue propyleneoxide was shown to proceed only in the presence of an enzyme (Fjellstedt et al. 1973). In rabbits, no effect was found on liver-glutathione and blood-glutathione levels, after 12 weeks of exposure to concentrations of ethylene oxide at 18, 90, or 450 mg/m³, for 5 days per week, 6hr per day (Yager & Bentz 1982). As ethylene oxide can react with chloride-ions, and this reaction is acid-catalysed, 2-chloroethanol might be expected to be a metabolite, especially after oral administration. However, neither 2-chloroethanol, not its metabolites have been found in the plasma, tissues, or urine of species exposed to ethylene oxide (Johnson 1967, Grunow & Altman 1982). Ehrenberg et al. (1974) found that an average of 74% of labelled ethyleneoxide inhaled by mice, was excreted in the urine within 24hr in the form of unidentified metabolites, and only 4% within the next 24hr. Thus, on the basis of this and previously presented excretion data, excretion of metabolites of ethylene oxide mainly takes place via the urine, within 24 hr following exposure.
Other information about bioaccumulation	Potential for accumulation negative (Sax 1986).
LD50 values to mammals in oral exposure, mg/kg	330 orl-rat (Smyth et al. 1941) 280–365 orl-mice (Woodard & Woodard 1971) > 10000 mg/kg, orl, 1,2-ethanediol 270 14d, orl-gpg 72 orl-rat (Sax 1986)
LD50 values to mammals in non-oral exposure, mg/kg	5210 1,2-ethanediol, rat, intravenous (Woodard & Woodard 1971) 290 ivn-mus (Sax 1986)
LC50 values to mammals in inhalation exposure, mg/m³	1500 4-hr, ihl-mus 1730 dog 2630 rat (Jacobson et al.1956)
LC50 values to mammals in inhalation exposure, ppm	4000 4hr, ihl-rat 836 4hr, ihl-mus 973 4hr, ihl-dog 1462 4hr, ihl-rat 960 4hr, ihl-dog (Sax 1986)
LDLo values to mammals in non-oral exposure, mg/kg	444 ivn-dog 100 ipr-mus 175 ivn-rbt (Sax 1986)

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TDLo values to mammals in non-oral exposure, mg/kg	225 ivn-mus, 10-12d preg, teratogenic 450 ivn-mus, 8-10d preg, teratogenic 450 ivn-mus, 10-12d preg, teratogenic 292 scu-mus, 95W-I, tumorigenic (Sax 1986)
TCLo values to mammals in inhalation exposure, mg/kg	3.6 ihl-rat, 24hr, 60d male, teratogenic (Sax 1986)
TCLo values to mammals in inhalation exposure, ppm	100 ihl-rat, 6hr, 6-15d preg, teratogenic 12500 ihl-hmn, 10s 500 ihl-wmn, 2min (Sax 1986)
Effects on the physiology of mammals	Acute exposures:(oral, intravenous and inhalation studies) In mortality studies, the lungs and nervous system are the main targets in rodents and dogs. In dynamic inhalation exposure studies on guinea-pigs (Waite et al.1930, Jacobson et al.1956) rats, mice and dogs, nasal irritation was the first clinical effect. Respiratory problems occured ranging from gasping to laboured breathing. Dogs exhibited laboured breathing, vomited, and suffered convulsions. Guinea-pigs, exposed to a concentration of 13000 mg ethylene oxide /m³, for 2.5hr, were found lying on their sides, unable to stand, and quiet. Gross pathological changes in animals that did not survive included moderate congestion in the lungs of dogs, minor patchy oedema in the lungs of rats, and congestion with oedema in the lungs of guinea-pigs. In rats, moderate congestion with petecchial haemorrhage of the trachea was also observed. Lobural pneumonia and hyperaemia of the liver and kidneys were observed in guinea-pigs. Parenchymatous changes in the kidney of guinea-pigs were seen at 2300 mg/m³. Ataxia, prostration, laboured breathing, and occasional toxic convulsions were effects shown by rats and mice at lethal oral or intravenous doses of ethyleneoxide (Woodard & Woodard 1971). Rabbits were exposed for 2hr via polyvinyl chloride endotracheal tubes containing 0–600 mg ethylene oxide /kg material. There were no deaths, but rabbits receiving the tubes with the highest residues showed increased incidences of hyperaemia, oedema, leukocyte infiltration, and epithelial erosion of the larynx and trachea (Star et al.1980). Acute effects on eyes and skin: Concentrations above 1% ethylene oxide established into the conjunctival sac of rabbits, caused reversible changes in conjunctiva such as hyperaemia and swelling, and irreversible opacity, both in the cornea and in the lens. Possible reaction products, 2-chloroethanol and 1,2-ethanediol, were less irritating to eye (McDonald et al.1973). Skin irritation with hyperaemia, oedema, and scar formation was observed from 6 min after application of pads of cotton, moistened with solutions of 100 or 500 g ethylene oxide /l water, on the shaved skin of rabbits, under a plastic cover (Hollingsworth et al. 1956). Liquid ethylene oxide is apparently without adverse effects on rabbit and human skin, on single mild exposures, if the material evaporates rapidly. If large amounts of material are involved, evaporation may cause sufficient cooling to cause a lesion similar to frost bite (Hine & Rowe 1981). Short-term studies: (inhalation exposure) Surviving rats showed increased relative lung weights after 26–27 weeks at 200 and 370 mg/m³. At 370 mg/m³, haemorrhages, hyperaemia, emphysema, and local alveolar collapse were observed in these lungs. Lungs of male rabbits also showed hyperaemia and slight oedema at 370 mg/m³. Gross respiratory tract irritation was apparent in all species at 1510 mg/m³. Delayed reversible effects were observed on the peripheral nervous system. Monkeys and rabbits exhibited paralysis of the hind legs at 370 mg/m³ and, together with rats, at 640 mg/m³. This was accompanied by atrophy of the muscles of the hind legs, except in rabbits at 370 mg/m³. The effects on the peripheral nervous system were investigated further in monkeys, and loss of both sensory and motor function was noted at levels 370 mg/m³ and 640 mg/m³. Significant increases in body weight were also observed in rats, at levels of 200 mg/m³ or more. Rats showed slight but significant increases in the relative weights of kidney and liver at 370 mg/m³ (Hollingsworth et al. 1956). Groups of mice were exposed to concentrations 0–425 mg/m³, for 6hr/day, and 5 days per week. The exposures lasted for 10–11 weeks. No effects were observed in relation to survival, body weight, clinical signs, white blood cell count, serum clinical chemistry, urinanalysis, and histopathology. At the highest exposure level, changes at terminal sacrifice included

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	an increased relative liver weight in female mice, and a decreased testicular weight in males. A decreased relative spleen weight was observed at 187 and 425 mg/m³ (Snellings et al. 1984a). Short-term studies: (oral exposure) Rats received 15 doses of 100 mg/kg ethylene oxide in 21 days. There was marked loss in body weight, gastric irritation, and slight liver damage (Hollingsworth et al. 1956). Long-term inhalation studies Rats were exposed to actual ethyleneoxide concentrations of 18–173 mg/m³ for 6hr per day, 5 days a week over 25 months. The mortality rates increased significantly from the 22nd and 23rd month, at the highest exposure. Body weights were depressed. In females, the relative liver weight were increased. Relative spleen weight were increased in rats that developed leukaemia. Haematological changes were found in rats at all doses. Non-neoplastic histopathological changes observed included an elevated frequency of focal fatty metamorphosis of the adrenal cortices in both sexes and bone marrow hyperplasia in females at 173 mg/m³. Also mild skeletal muscular atrophy was observed.
Effects on the reproduction of mammals	Rats and guinea-pigs were exposed to vapour concentrations of 370 and 640 mg ethylene oxide /m³, for 7hr per day, 5 days per week, for up to 32 weeks. Among other effects, degeneration of testes tubules was observed at the higher exposure level in guinea-pigs, while at 370 mg/m³, there was a decrease in the relative weights of testes in rats and guinea-pigs, which was not statistically significant (Hollingsworth et al.1956). Significantly decreased absolute testicular weights were observed in mice exposed to ethylene oxide at a concentration of 425 mg/m³, for 6hr/day, 5 days per week, over 10–11 weeks (Snellings et al. 1984a). However the testicular effects may have been secondary to toxic effects (e.g., growth inhibition). Rats exposed repeatedly to concentrations of ethyleneoxide of up to 182 mg/m³, for 6hr/day, 5 days per week, over 25 months, did not show any histopathological effects on the reproductive tissues (Snellings et al. 1981). When monkeys were exposed to concentrations of ethylene oxide at 90 and 180 mg/m³, for 7hr/day, 5 days per week, over 2 years, spermatogenic functions were found to differ from those of controls. At both exposure levels, sperm motility and sperm count were decreased and the sperm drive range was increased, but there was no increase in effect with increase in dose. The incidence of abnormal sperm heads did not change (Lynch et al. 1984c). Rats were exposed to concentrations of ethylene oxide of 18, 58, or 173 mg/m³, for 6hr/day, 5 days per week, over 12 weeks. After mating females were further exposed for 7 days/week, up to 3 weeks after delivery, with the exception of the first 5 days of lactation. Effects on the reproductive performance were detected. The number of pups per litter was decreased at 173 mg/m³, as well as the number of implantation sites per female, and the number of fetuses born per implantation site. The number of females with a gestation period longer then 22 days was also increased at this concentration, but no effects were noted on the average length of the gestation period. Neither parents nor pups showed signs of toxicity from ethylene oxide. The percentages of pregnant females and fertile males were not affected (Snellings et al. 1982a). Short-term studies: (inhalation exposure) Guinea-pigs, rabbits, and monkeys tolerated 90 and 200 mg/m³, and rats tolerated exposure to 90 mg/m³ without adverse effects on general appearance, behaviour, mortality rate, growth, body and organ weight, gross and histopathology. Rats showed eleveted mortality rates from 370 mg/m³, rabbits from 640 mg/m³, and all exposed animals died at 1510 mg/m³. Secondary respiratory infection caused the deaths of an appreciable number of rats and mice in these studies (Hollingsworth et al.1956).

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	The potential of ethylene oxide to cause teratogenic or adverse reproductivity effects has been examined in 4 animal species (mice, rats, rabbits, and monkeys) by 2 routes of administration. Results from these studies showed that ethylene oxide is toxic to reproductive function in both males (reduced sperm number and sperm motility, and an increased time to traverse a linear path) and females (depression of fetal weight gain, fetal death, and fetal malformation). The levels needed to produce these fetal effects approach or equal the dose needed to produce maternal toxicity. The results of animal studies suggest possible reproductive impairment in human males but are inadequate for assessing the fetal risk. Data on reproductive effects in human beings are insufficient; one study (Hemminki et al. 1982) suggests an increase in spontaneous abortion rate in women occupationally exposed to ethylene oxide. However, the reported time-weighted average air concentrations may not reflect the exposure levels that induced the effect (WHO 1985).
Health effects	Moderately toxic by inhalation. Characteristic ether odour irritating in high concentrations. Anesthetic. Can cause pulmonary edema. Max allowable concentration is 100 ppm. 3000 ppm may be tolerated for 60 minutes max. 50000–100000 ppm fatal within few minutes. Strong irritant and and inhalative poison. – Chronic irritant (Sax 1986). Skin and eye irritation data: skn, hmn, 1%, 7 s; eye, rbt, 18 mg, 6hr, moderate (Sax 1986).
Carcinogenicity	Ethylene oxide has induced following effects: Inhalation exposure: – neoplasms in rats (Snellings et al. 1981, 1984b) – increased incidence of mononuclear cell leukaemia in rats (Snellings et al. 1981, 1984b, Lynch et al. 1984a) – primary brain tumours in rats (mainly gliomas and malignant reticular tumours) (Snellings et al. 1981, 1984b) – peritoneal mesotheliomas in rats, originating from the testicular mesothelium and of mixed-cell gliomas in the brain (Lynch et al. 1984a) Oral exposure: – elevated incidences of tumours in the forestomach in rats – elevated incidences of squamous cell carcinomas in rats – invasive growth, metastases, fibrosarcomas in rats – elevated incidences of hyperplasia, hyperkeratosis, papillomas and carcinomas in the forestomach of rats (Dunkelberg 1982). Subcutaneous exposure: – elevated incidence of tumours only at the injection site though the mortality rate was increased (mice). – increased incidence of sarcomas, mainly fibrosarcomas in mice (Dunkelberg 1981) Dermal exposure: – no skin tumours were found, nor was there any sign of skin irritation, when mice received ethyleneoxide in acetone, brushed on the clipped dorsal uncovered skin. It was assumed that ethyleneoxide evaporated rapidly from the skin (Van Duuren et al. 1965)
Mutagenicity	Almost all reports available demonstrate the mutagenic action of ethylene oxide.Ethylene oxide is an alkylating agent.It has induced gene mutations in all plants, bacteria, fungi, insects, and mammalian cells investigated in vitro, with and without metabolic activation. Chromosome damage and sister chromatid exchanges were observed in plants, insects, and mammalian somatic cells exposed in vivo and in vitro (Fomenko & Strekalova 1973, Embree & Hine 1975, Strekalova et al. 1975, Appelgren et al.1977, Cumming & Michaud 1979, Generoso et al. 1980, Pero et al. 1981, Lyarskii et al. 1983). Negative results were observed on a few occasions only (Appelgren et al. 1977, Kligerman et al. 1983). Known to cause mutations and chromosome aberrations. Positive both in barley spikes and neurospora and reversions (Sax 1986).

	Mutagen data: mmo, sat, 0.040 mmol/plate; cyt, dmg, par, 55 mmol/l; mmo, nsc, 140 mmol/l, 10 min; mnt, rat, ivn, 200 mg/kg; cyt, rat, ihl, 0.001 mg/l, 17 weeks; dlt, rat, ihl, 1000 ppm, 4hr; dns, mus, ihl, 300 ppm; dlt, mus, ipr, 150 mg/kg; trn, mus, ipr, 30 mg/kg, 25D-l; sce, rbt, ihl, 50 ppm, 12W-I (Sax 1986).	
Teratogenicity	Rats were exposed to concentrations of ethylene oxide of 18, 58, or 173 mg/m³, for 6hr/day, on days 6–15 of gestation. Maternal behaviour was normal, and there were no deaths. The only effect on the fetuses was a 5–8% decrease in weight at 180 mg/m³ (Snellings et al. 1982b.) Rats were exposed to concentrations of ethylene oxide of 0 and 270 mg/m³, for 7hr/day, on days 7–16 of gestation (group 1) or on days 1–16 of gestation (group 2) or during 3 weeks before mating (5 days per week), and on days 1–16 of gestation (group 3). No dams died, but body weights were decreased in group 3. In all exposed groups, the relative and absolute weight of kidney and spleen were increased. The results of histopathological examination did not show any abnormalities. There was a significant increase in resorptions per litter and per implantation site in group 3, with no significant effect on the number of implants, live fetuses, and pregnancies. In all exposed groups, weights and lengths of the fetuses were decreased. Reduced ossification of sternebrae and primary skull was observed (Hackett et al. 1982). Female mice received, intraveneously, doses of 0, 75, or 150 mg ethylene oxide /kg body weight in an aqueous dextrose solution on days 4–6, 6–8, 8–10, or 10–12 of pregnancy. Dams exposed on days 6–8 of pregnancy did not show toxic signs. In the other groups, at the highest dose, toxic signs such as weakness, laboured respiration, and tremor were observed with a mortality rate of 19–48%. In the group without signs of maternal toxicity, fetotoxicity was observed at 150 mg/kg, as shown by a 20% decrease in mean fetal weight.Fetal malformation were shown in 19.3% of fetuses in exposed litters compared with 2% in control groups. These malformations were mainly fused cervical arches. In addition, fused thoracic arches, scrambled and fused sternebrae, and fused, branched, or missing thoracic ribs were observed (Laborde & Kimmel 1980).	
Maximum longterm immission concentration in air for plants, mg/m³	4	VDI 2306
Maximum longterm immission concentration in air for plants, ppm	2	VDI 2306
LC50 values to crustaceans, mg/l	212	48hr, Daphnia magna (Conway et al.1983) > 10000 mg/l, 1,2-ethanediol 100 mg/l, 2-chloroethanol
LC50 values to fishes, mg/l	84	96hr, Pimephales promelas (Conway et al. 1983) > 10000 mg/l, 1,2-ethanediol 90 mg/l, 2-chloroethanol
	90	24hr, Carassius auratus (Bridie et al. 1979a) > 5000 mg/l, 1,2-ethanediol

1021 • Ethylene thiourea 96-45-7

Synonyms	2-Mercapto imidazoline	
Water solubility, mg/l	> 10000	(MITI 1992)
Melting point, °C	198	(MITI 1992)

Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.2–0.3 6w, Cyprinus carpio, conc 1 mg/l < 1.8 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
EC50 values to microorganism, mg/l	2447 15 min Microtox (Govers et al. 1986)
EC50 values to algae, mg/l	6600 rpd, act, 96hr, Chlorella pyrenoidosa (Leeuwen et al. 1985)
LC50 values to crustaceans, mg/l	26 48hr, Daphnia magna (Leeuwen et al. 1985)
LC50 values to fishes, mg/l	7500 96hr, Poecilia reticulata (Leeuwen et al. 1979) > 1000 48hr, Oryzias latipes (MITI 1992)

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1022 • Ethylenebromide 106-93-4

Synonyms	1,2-Dibromoethane EDB
Use	Scavenger for lead in gasoline; grain and fruit fumigant; general solvent; waterproofing preparations. Petrol additive; fumigant.
State and appearance	Colourless liquid.
Molecular weight	187.88
Vapour pressure, mmHg	11 20 °C
Water solubility, mg/l	4.31 30 °C
Melting point, °C	93 (MITI 1992)
Boiling point, °C	131.6 (MITI 1992)
Log octanol/water coefficient, log Pow	4.3 (Anon. 1988)
Henry's law constant, Pa x m³/mol	66000 (Anon. 1988) 70.76 calc. (Yaws et al. 1991)
Mobility	Equilibrium distribution: *mass %* air 99.98 water 0.00 solid 0.02 (Anon. 1988).
Other reactions in atmosphere	Is resistant to atmospheric oxidation by peroxides and ozone, typically the half-life is in excess of 100 days (Verschueren 1983).
Total degradation in soil	Degradation in soil is about 2 months (Verschueren 1983).
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

Bioconcentration factor, fishes	1.6–3.2 < 3.5–14.9	6w, Cyprinus carpio, conc 150 000 mg/l 6w, Cyprinus carpio, conc 15 000 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987) (1,2-dibromoethane).	
LD50 values to mammals in oral exposure, mg/kg	108 55	orl-rat orl-rbt (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	300	skn-rat, skn-rbt (Lewis & Sweet 1984)
LCLo values to mammals in inhalation exposure, ppm	400	2hr, ihl-rat (Lewis & Sweet 1984)
Carcinogenicity	NCI and NTP carcinogenesis bioassays completed: results positive; mus, rat (Lewis & Sweet 1984).	
LD50 values to birds in oral exposure, mg/kg	79	orl-ckn (Lewis & Sweet 1984)
LC50 values to fishes, mg/l	183	48hr, Oryzias latipes (MITI 1992)

1023 • Ethylenediamine 107-15-3

Synonyms	1,2-Ethanediamide 1,2-Diaminoethane	
Sumformula of the chemical	C2H8N2	
Purity, %	100 76 91	anhydrous solution 91-93% solution
Use	Medicine; neutralizing oils; corrosion inhibitor in antifreeze solutions; textile; lubricant. Shellac; solvent; emulsifier; rubber; latex.	
State and appearance	Colourless liquid. Will dissolve.	
Odour	Quality: ammonical, musty Hedonic tone: unpleasant Threshold odour concentration absolute: 1.0 ppm 50% recognition: 3.4 ppm 100% recognition: 11.2 ppm Odour index 100% recognition: 1 178 (Hellman & Small 1974).	
Molecular weight	60.1	
Specific gravity (water=1)	0.898	
Vapour density (air=1)	2.1	
Vapour pressure, mmHg	10.7 20 53	20 °C 33 °C 53 °C
Water solubility, mg/l	> 100 000 mg/l	(MITI 1992)
Melting point, °C	10.8	(MITI 1992)
Boiling point, °C	116.5	(MITI 1992)
Flashing point, °C	43.3	

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Other physicochemical properties	Flammability: moderate. Compustion with moderate heating. Toxic combustion products: extreme danger. Explosiveness: Reactive – combines chemically with many materials. Highly reactive. Miscible.
Total degradation in water	Biodegradation: 93–95% (NH_3) by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Other information about degradation	Biodegrades quite rapidly (Sax 1986).
LD50 values to mammals in oral exposure, mg/kg	1160 orl-rat 470 orl-gpg (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	656 skn-rbt (Lewis & Sweet 1984) 76 ipr-rat 200 ipr-mus 424 scu-mus 730 skn-rbt (Sax 1986)
LC50 values to mammals in inhalation exposure, mg/m³	300 ihl-mus (Lewis & Sweet 1984)
LDLo values to mammals in non-oral exposure, mg/kg	150 scu-rat 100 ivn-dog 500 scu-rbt (Sax 1986)
LCLo values to mammals in inhalation exposure, ppm	4000 8hr, ihl-rat (Sax 1986)
TCLo values to mammals in inhalation exposure, ppm	200 ihl-hmn (Lewis & Sweet 1984)
Health effects	Allegric dermatitis (Sax 1986). Direct contact: Severe eye and skin burns, respiratory distress (Sax 1986). General sensation: Strong ammonia odour. Skin irritation grade 6-necrosis undiluted; forms alkaline solution. Eye irritation grade 8-severe burns. Can be absorbed through skin. Irritant and allergen (Sax 1986). Acute hazard level: Moderately toxic via all routes. Emits toxic vapours when heated to decomposition (Sax 1986). Chronic hazard level: Can sensitize skin. Chronic exposure to sublethal levels can prove moderately toxic via all routes (Sax 1986). Skin and eye irritation data: skn, rbt, 450 mg, open, moderate; skn, rbt, 10 mg, 24hr, severe; eye, rbt, 0.675 mg, severe (Sax 1986).
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 0.85 mg/l (Bringmann & Kühn 1980a).
Effects on wastewater treatment	100–300 mg/l nonsubstrate limiting to anaerobic processes (Sax 1986).
EC50 values to algae, mg/l	100 rpd, act, 96hr, Chlorella pyrenoidosa (Leeuwen et al. 1985)

LOEC values to algae, mg/l	0.08 0.85	rpd, schr, Microcystis aeruginosa (Bringmann & Kuhn 1976) rpd, schr, Scenedesmus quadricauda (Bringmann & Kuhn 1980a)
LC50 values to crustaceans, mg/l	0.88 27	48hr, Daphnia magna (Isensee et al. 1973) 48hr, Daphnia magna (Leeuwen et al. 1985)
LC50 values to fishes, mg/l	230 115.7 275	48hr, Salmo gairdneri (Woodwiss & Fretwell 1974) 96hr, Pimephales promelas (Curtis & Ward 1981) 96hr, Poecilia reticulata (Leeuwen et al. 1985)
Other information about water organisms	60 mg/l, 24hr, chub, killed; 200 mg/l, Escherichia coli, adverse response; 8 mg/l, Daphnia, toxic, 23 °C; 30 mg/l, Microregma, adverse response; 20 mg/l, Scenedesmus, toxic; > 100 mg/l, 72hr, shiners, no toxic effect (Sax 1986). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 0.85 mg/l protozoa (Entosiphon sulcatum): 1.8 mg/l (Bringmann & Kühn 1980a).	
Other information	Poses BOD problem (Sax 1986). Air pollution high (Sax 1986). Forms alkaline solution from dissociation of amine group which form ammonium ions, subject to biodegradation (Sax 1986).	

1024 • Ethylenediamine tetraacetate 60-00-4

Synonyms	EDTA	
LOEC values to algae, mg/l	11	rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
LC50 values to fishes, mg/l	159	96hr, Lepomis macrochirus (Batchelder et al. 1980)
	59.8	96hr, Pimephales promelas (Curtis & Ward 1981)
		* Cu-chelate
	555	96hr, Lepomis macrochilus (Batchelder et al. 1980)
		* Diammonium salt
	2340	96hr, Lepomis macrochilus
		* Tetra-ammonium chelate
	705	96hr, Lepomis macrochilus
		* Mg-chetate
	2520	96hr, Lepomis macrochilus
		*Tetra-Na-salt
	486	96hr, Lepomis macrochilus
		* Zn-chelate
	685	96hr, Lepomis macrochilus

1025 • Ethyleneglycol 107-21-1

Synonyms	Glycol 1,2-Ethanediol 1,2-Dihydroxyethane 1,2-Ethandiol Ethane-1,2-diol Ethylene alcohol Ethylene dihydrate Ethyleneglycol Glycol alcohol Monoethylene glycol 2-Hydroxyethanol
Sumformula of the chemical	C2H6O2
Use	Solvent; antifreeze agent, heat transfer agents and in polyester fiber and film manufacture.
Molecular weight	62.08
Vapour pressure, mmHg	0.0878 at 25 °C (Riddick et al. 1986)
Water solubility, mg/l	> 100 000 (MITI 1992)
Melting point, °C	-12.6 (MITI 1992)
Boiling point, °C	197.6 (MITI 1992)
Log octanol/water coefficient, log Pow	-1.36 (Hansch & Leo 1985)
Henry's law constant, Pa x m³/mol	0.0061 (Howard 1990)
Volatilization	Relative volatility (nBuAc=1) = 0.01
Other reactions in atmosphere	Ethylene glycol reacts with hydroxyl radicals in the atmosphere. Based on a hydroxyl radical concentration of 1000000 molecules/cm³, a half-life of ethylene glycol is about 1 day in the atmosphere. (Howard 1990)
Photochemical degradation in water	Photooxidation in aqueous systems will not be significant. (Howard 1990)
Chemical oxygen demand, g O2/g	1.29 5 days (Bridie et al. 1979)
Biochemical oxygen demand, g O2/g	0.47 5 days (Bridie et al. 1979)
Total degradation in water	Ethylene glycol will readly biodegrade in water, half-life several days. It is not expected to adsorb to sediment. (Howard 1990) Biodegradation: 83–96% by BOD period: 14d substance: 100 mg/l sludge 30 mg/l (MITI 1992).
Other information about degradation	Degradation was essentially complete in < 1–4 days although 100% theoretical biological oxygen demand may not be realized for several weeks. (Howard II 1990) In a river die-away test, degradation was completed in 3 days at 20 °C and 5–14 days at 8 °C. (Evans & David 1974)
Bioconcentration factor, fishes	10 3d, Golden ide (Freitag et al. 1985)
Bioconcentration factor, algae	190 1d, Chlorella fusca (Freitag et al. 1985)

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LD50 values to mammals in oral exposure, mg/kg	5840	orl-rat
	1650	orl-cat
	5500	orl-dog
	6610	orl-gpg
	7500	orl-mus
	4700	orl-rat (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	5614	ipr-mus
	5010	ipr-rat
	1000	ipr-rbt
	3000	ivn-mus
	3260	ivn-rat
	2800	scu-rat
	9530	skn-rbt (Sweet 1987)
LDLo values to mammals in oral exposure, mg/kg	786	orl-hmn
	398	orl-hmn (Sweet 1987)
LDLo values to mammals in non-oral exposure, mg/kg	3300	intramuscular-rat
	5500	intramuscular-rbt (Sweet 1987)
	2000	scu-cat
	5000	scu-gpg
	2700	scu-mus (Sweet 1987)
TDLo values to mammals in oral exposure, mg/kg	7500	orl-mus, 6-15d preg. effects on embryo or fetus specific developmental abnormalities
	7500	orl-mus, 6-15d preg. specific developmental abnormalities
	84	orl-mus, 1-21d preg. effects on newborn
	88720	orl-mus, 7-14d preg. effects on fertility and newborn
	15	orl-mus, 6-15d preg. maternal effects, eff. on fertility
	50	orl-rat, 6-15d preg. specific developmental abnormalities
	10	orl-rat, 6-15d preg. specific developmental abnormalities
	12500	orl-rat, 6-15d preg. specific developmental abnormalities
	25	orl-rat, 6-15d preg. maternal effects, eff. on fertility eff. on embryo of fetus
	50	orl-rat, 6-15d preg. effects on fertility (Sweet 1987)
	5500	orl-child (Sweet 1987)
TCLo values to mammals in inhalation exposure, mg/kg	10000	ihl-hmn (Sweet 1987)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): > 10000 mg/l (Bringmann & Kühn 1980a)	
LOEC values to algae, mg/l	2000	rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)

EF

LC50 values to fishes, mg/l	> 5000 24hr, Carassius auratus (Bridie et al. 1979) 49300 7d, Poecilia reticulata (Könemann 1979)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): > 10000 mg/l protozoa (Entosiphon sulcatum): > 10000 mg/l (Bringmann & Kühn 1980a)

1026 • Ethyleneglycol acetate 111-55-7

Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 875 mg/l (Bringmann & Kühn 1980a).
LOEC values to algae, mg/l	9 rpd, act, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
LC50 values to fishes, mg/l	78 96hr, Menidia audens 90 96hr, Lepomis macrochirus (Dawson et al. 1977)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 9 mg/l protozoa (Entosiphon sulcatum): 34 mg/l (Bringmann & Kühn 1980a)

EF

1027 • Ethyleneglycol monoethylether 110-80-5

Synonyms	2-Ethoxyethanol
Sumformula of the chemical	C4H10O2
Use	Solvent for nitrocellulose, natural and syntethetic resins; mutual for formulation of soluble oils; lacquers and lacquer thinners, dyeing and printing textiles, varnish removers, cleaning solutions, leather, anti-icing additive for aviation fuels.
State and appearance	Colourless liquid.
Odour	Practically odourless.
Specific gravity (water=1)	0.9311
Melting point, °C	-70 (MITI 1992)
Boiling point, °C	135 (MITI 1992)
Flashing point, °C	48.9
Volatilization	Relative volatility (nBuAc=1) = 0.38 Miscible with hydrocarbons, water, autoign temperature 237 °C. Combustible.
Chemical oxygen demand, g O2/g	1.92 5 days (Bridie et al. 1979)
Biochemical oxygen demand, g O2/g	1.03 5 days (Bridie et al. 1979)
Total degradation in water	Biodegradation: 63–83% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	3000 orl-rat

LC50 values to fishes, mg/l	> 10000	96hr, Lepomis macrochirus Menidia audens (Dawson et al. 1977)
	> 5000	24hr, Carassius auratus (Bridie et al. 1979)
	16400	7d, Poecilia reticulata (Könemann 1979)

1028 • Ethyleneglycol monomethylether 109-86-4

Synonyms	2-Methoxyethanol	
Sumformula of the chemical	C3H9O2	
Use	Solvent for nitrocellulose, cellulose acetate, alcohol-soluble dyes, natural and synthetic resins, solvent mixtures, lacquers, enamels, varnishes, leather, perfume fixtive, wood stains, sealing moisture-proof cellophane, jet fuel deicing additive.	
State and appearance	Colourless liquid, stable.	
Odour	Mild agreeable odour.	
Specific gravity (water=1)	0.9663	
Water solubility, mg/l	Infinite > 100000	 (MITI 1992)
Melting point, °C	< -10	(MITI 1992)
Boiling point, °C	122–126	(MITI 1992)
Flashing point, °C	43.3	
Volatilization	Relative volatility (nBuAc=1) = 0.70	
	Miscible with hydrocarbons, alcohols, ketones, glycols and water. Autoignition temperature 288 °C. Combustible.	
Chemical oxygen demand, g O2/g	1.69	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g O2/g	0.12	5 days (Bridie et al. 1979)
Total degradation in water	Biodegradation: 73–94% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
LD50 values to mammals in oral exposure, mg/kg	2140	
LOEC values to algae, mg/l	100	rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to fishes, mg/l	> 10000	96hr, Lepomis macrochirus Menidia audens (Dawson et al. 1977)
	15520	96hr, Salmo gairdneri (Verschueren 1983)
	17400	7d, Poecilia reticulata (Könemann 1979)
	> 5000	24hr, Carassius auratus (Bridie et al. 1979)

EF

1029 • Ethyleneglycol monomethylether acetate 110-49-6

Synonyms	Methylcellosolveacetate Methylglycol acetate Glycomonomethylether acetate 2-Methoxyethyl acetate	
Use	Solvent.	
Melting point, °C	-62	(MITI 1992)
Boiling point, °C	156.3	760 mmHg (MITI 1992)
Volatilization	Relative volatility (nBuAc=1) = 0.31	
Chemical oxygen demand, g 02/g	1.6	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.49	5 days (Bridie et al. 1979)
Total degradation in water	Biodegradation: 86.90% by BOD period: 12d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
LD50 values to mammals in oral exposure, mg/kg	3390	orl-rat
LC50 values to fishes	45 40 190	96hr, Lepomis macrochirus 96hr, Menidia audens (Dawson et al. 1977) 24hr, Carassius auratus (Bridie et al. 1979)

1030 • Ethylfenthion 1716-09-2

Other information about mammals	LDfr = 87.5 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

1031 • Ethylglycol acetate 111-15-9

Synonyms	2-Ethoxyethyl acetate	
Use	Solvent.	
Water solubility, mg/l	229000	20 °C
Boiling point, °C	156	
Volatilization	Relative volatility (nBuAc=1) = 0.21	
Chemical oxygen demand, g 02/g	1.76	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.74	5 days (Bridie et al. 1979)
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	5100	orl-rat

EF

LC50 values to fishes, mg/l	98 107–141 42.2 44.8 160	96hr, Branchydanio rerio 48hr, Leuciscus idus (Wellens 1982) 96hr, Pimephales promelas 96hr, Ictalurus punctatus (Holcombe et al. 1984) 96hr, Carassius auratus (Bridie et al. 1979)
Other information about water organisms	LC50, 65.2 mg/l, 96hr, snail (Holcombe et al. 1984)	

1032 • N-(2-Ethylhexyl)-1-isopropyl-4-methylbicyclo(2,2,2)- octa-5-ene-2,3-dicarboxyimide 13358-11-7

Sumformula of the chemical	C22H35NO2	
Water solubility, mg/l	0.04	(MITI 1992)
Boiling point, °C	175	0.1 mmHg (MITI 1992)
Log octanol/water coefficient, log Pow	5.96	(MITI 1992)
Total degradation in water	Biodegradation: 0–2% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	637–2140 331–1540	8w, Cyprinus carpio, conc 0.02 mg/l 8w, Cyprinus carpio, conc 0.002 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be accumulated on a medium level (Anon. 1987).	
LC50 values to fishes, mg/l	4.09	48hr, Oryzias latipes (MITI 1992)

1033 • 2-Ethylhexyl alcohol 104-76-7

Synonyms	2-Ethyl-1-hexanol	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LC50 values to fishes, mg/l	32–37	96hr, Salmo gairdneri (Dave & Lindman 1978)

1034 • 2-Ethylhexyl amine 103-09-3

Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 82 mg/l (Bringmann & Kühn 1980a).	
LOEC values to algae, mg/l	0.36 0.02	rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a) rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 0.36 mg/l protozoa (Entosiphon sulcatum): 12 mg/l (Bringmann & Kühn 1980a).	

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1035 • 2-Ethylhexyl glycidyl ether 2461-15-6

Synonyms	1-(2,3-Epoxypropoxy)-2-ethylhexane	
Chemical oxygen demand, g 02/g	2.46	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.14	5 days (Bridie et al. 1979)
LC50 values to fishes, mg/l	14	24hr, Carassius auratus (Bridie et al. 1979)

1036 • 2-Ethylhexyldiphenyl phosphate 1241-94-7

Sumformula of the chemical	C20H2704P	
Water solubility, mg/l	< 10	(MITI 1992)
Melting point, °C	-54	(MITI 1992)
Boiling point, °C	375	760 mmHg (MITI 1992)
Log octanol/water coefficient, log Pow	> 3.78	(MITI 1992)
Total degradation in water	Biodegradation: 0–2% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	433–735 194–426	8w, Cyprinus carpio, conc 0.1 mg/l 8w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
LC50 values to fishes, mg/l	17.7	48hr, Oryzias latipes (MITI 1992)

1037 • 2-Ethylhexylvinylether 103-44-6

Sumformula of the chemical	C10H200	
EINECS-number	2031114	
Water solubility, mg/l	1.8	(MITI 1992)
Melting point, °C	< -10	(MITI 1992)
Boiling point, °C	83–85, 38–40 mmHg	(MITI 1992)
Log octanol/water coefficient, log Pow	5.04	(MITI 1992)
Total degradation in water	Biodegradation: 4–10% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	1200–2550 345–837	8w, Cyprinus carpio, conc 0.025 mg/l 8w, Cyprinus carpio, conc 0.0025 mg/l (MITI 1992)
LC50 values to fishes, mg/l	2.92	48hr, Oryzis latipes (MITI 1992)

EF

1038 • 5-Ethylidene-2-norbornene

16219-75-3

Synonyms	Ethylidene norbornene
Odour	Quality: sweet, aromatic Hedonic tone: unpleasant to pleasant Threshold odour concentration absolute: 0.02 ppm 50% recognition: 0.073 ppm 100% recognition: 0.073 ppm Odour index 100% recognition: 75 616 (Hellman & Small 1974).
Water solubility, mg/l	8.9 (MITI 1992)
Boiling point, °C	144–148 (MITI 1992)
Log octanol/water coefficient, log Pow	3.82 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	70–160 8w, Cyprinus carpio, conc 0.1 mg/l 61–159 8w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	9.21 48hr, Oryzias latipes (MITI 1992)

1039 • n-Ethylmorpholine

100-74-3

Synonyms	N-Ethyl morpholine
Use	Solvent.
Odour	Quality: ammoniacal Hedonic tone: unpleasant to pleasant Threshold odour concentration absolute: 0.08 ppm 50% recognition: 0.25 ppm 100% recognition: 0.25 ppm Odour index 100% recognition: 26 280 (Hellman & Small 1974).
Boiling point, °C	138–139
LD50 values to mammals in oral exposure, mg/kg	1780 orl-rat

1040 • o-Ethylnitrobenzene

612-22-6

Synonyms	2-Ethylnitrobenzene
Sumformula of the chemical	C8H9O2N
Water solubility, mg/l	240 (MITI 1992)

EF

Log octanol/water coefficient, log Pow	2.58 (MITI 1992)
Total degradation in water	Biodegradation: 5% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	6.6–25 6w, Cyprinus carpio, conc 0.01 mg/l < 3.5–13 6w, Cyprinus carpio, conc 0.001 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	37 48hr, Oryzias latipes (MITI 1992)

1041 • 2-Ethylphenol 90-00-6

Sumformula of the chemical	C8H10O
Log octanol/water coefficient, log Pow	2.47 (Sangster 1989)

1042 • 3-Ethylphenol 620-17-7

Sumformula of the chemical	C8H10O
Log octanol/water coefficient, log Pow	2.5 (Sangster 1989)

1043 • 4-Ethylphenol 123-07-9

Sumformula of the chemical	C8H10O
Log octanol/water coefficient, log Pow	2.5 (Sangster 1989)
Other information about water organisms	Tetrahymena pyriformis; 76.06 mg/l, 2d, EC50, grw (Schultz 1987).

1044 • Ethylpropionate 105-37-3

Synonyms	Propanoic acid, ethyl ester
Sumformula of the chemical	C5H10O2
Log octanol/water coefficient, log Pow	1.21 (Sangster 1989)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 270 mg/l (Bringmann & Kühn 1980a).
LOEC values to algae, mg/l	14 rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
NOEC values to algae, mg/l	140 rpd, schr, Selenastrum capricornutum (Slooff et al. 1983)

LC50 values to crustaceans, mg/l	170 70 45 120 167	48hr, Daphnia magna 48hr, Daphnia pulex 48hr, Daphnia cucullata (Canton & Adema 1978) 48hr, Asellus aquaticus (Slooff 1983) 48hr, Gammarus pulex (Slooff 1983)
LC50 values to fishes, mg/l	56	48hr, Salmo gairdneri (Slooff et al. 1983)
Other information about water organisms	LC50, 48hr, 180 mg/l, Tubificidae LC50, 48hr, 65 mg/l, Chironomus gr. thummi LC50, 48hr, 210 mg/l, Erpobdella octoculata LC50, 48hr, 170 mg/l, Lymnaea stagnalis LC50, 48hr, 1000 mg/l, Dugesia cf. lugubris LC50, 48hr, 340 mg/l, Hydra oligactis LC50, 48hr, 600 mg/l, Corixa punctata LC50, 48hr, 243 mg/l, Ischura elegans LC50, 48hr, 20 mg/l, Nemoura cinerea LC50, 48hr, 194 mg/l, Cloeon dipterum (Slooff 1983). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 14 mg/l protozoa (Entosiphon sulcatum): 560 mg/l (Bringmann & Kühn 1980a).	

1045 • Ethylpyridine 536-72-4

Other information about water organisms	EC50 (60hr), rpd, 210 mg/l, Tetrahymena pyriformis (Schultz & Mouton 1985).

1046 • Ethylstyrene 28106-30-1

Sumformula of the chemical	C10H12	
Water solubility, mg/l	7.8 1.1	m- (MITI 1992) p- (MITI 1992)
Melting point, °C	< -10	(MITI 1992)
Log octanol/water coefficient, log Pow	4.11 4.19	m- (MITI 1992) p- (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	289–569 308–573 375–619 362–576	m-, 6w, Cyprinus carpio, conc 0.025 mg/l p-, 6w, Cyprinus carpio, conc 0.024 mg/l m-, 6w, Cyprinus carpio, conc 0.0025 mg/l p-, 6w, Cyprinus carpio, conc 0.0025 mg/l (MITI 1992)
LC50 values to fishes, mg/l	3.45	48hr, Oryzias latipes (MITI 1992)

EF

1047 • Eulan 3687-70-5

Synonyms	3,4-Dichlorobenzyl)triphenylphosninium chloride Eulan NK Eulan NKU
Use	Treatment of textiles.
Molecular weight	457.77
LD50 values to mammals in oral exposure, mg/kg	2000 orl-mam (Lewis & Sweet 1984)
LC50 values to fishes, mg/l	0.13 96hr, Salmo gairdneri 0.5 96hr, Carassius auratus 0.1 96hr, Lepomis macrochirus (Könemann 1979)

1048 • Faneron Combi 500 FW * (Bromophenoxim) 13181-17-4 (Terbutylazine) 5915-41-3

Chemicals in the product	Bromophenoxim 330 g/l; Terbutylazine 170 g/l
Use	Herbicide.
Way to effect	Photosynthesisinhibitor, contact function, systemic. (PESREG)
Instructions for handling	Stable max. 2 years at 20 °C, subject to storage in closed original containers. (PESREG)
State and appearance	Flowable aqueous suspension Yellow to brown flowable paste (PESREG)
Particle size, mm	0.015 min. 95% < 15 microns (PESREG) Behaviour in water: suspensible. Non-flammable. Non currosive.(PESREG)
LD50 values to mammals in oral exposure, mg/kg	1921 orl-rat (PESREG)
LD50 values to mammals in non-oral exposure, mg/kg	> 3100 idr-rat (PESREG)
LC50 values to mammals in inhalation exposure, mg/m³	> 800 4hr, ihl-rat (PESREG)
LC50 values to fishes, mg/l	0.6 96hr, Salmon trutta fario 0.53 96hr, Ictalurus melas (PESREG)

1049 • Fenaminphos 22224-92-6

Half-life in soil, days	10 (Li et al. 1990)
Other information about mammals	ALD = 18 mg/kg, act, orl, deer mouse; LDfr = 100 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

EF

1050 • Fenbutatin oxide

13356-08-6

Synonyms	Vendex Torque SD 14114	
Use	Active ingredient in acaricides.	
Molecular weight	1052.76	
LD50 values to mammals in oral exposure, mg/kg	2630	orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	1000	skn-rat (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	> 100 > 100	orl-Agelaius phoeniceus orl-Sturnus vulgaris (Schafer et al. 1983)
LC50 values to fishes, mg/l	0.0015 0.016 0.017	96hr, cat fish (Nikunen et al. 1986) 96hr, Pimephales promelas 96hr, Salmo trutta (Nikunen et al. 1986)

EF

1051 • Fenchlorphos

299-84-3

Synonyms	0,0-Dimethyl-0-(2,4,5-trichlorophenyl)-phosphorothioate Ronnel	
Use	Insecticide.	
Molecular weight	321.54	
Vapour pressure, mmHg	0.0008	25 °C
Water solubility, mg/l	40	room temperature
Melting point, °C	40–42	
LD50 values to mammals in oral exposure, mg/kg	906 420	orl-rat orl-rbt (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	1000 400	skn-rbt unk-mam (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	80 500 75.0–80.0 353–375	orl-bwd (Lewis & Sweet 1984) orl-trk (Lewis & Sweet 1984) orl-Agelaius phoeniceus orl-Sturnus vulgaris (Schafer et al. 1983)
LC50 values to crustaceans, mg/l	0.002 0.0057	act, Daphnia pulex (Frear & Boyd 1967) act, Daphnia magna (Kenaga 1979)
LC50 values to fishes, mg/l	0.74 1 0.31	Salmo gairdneri Lepomis macrochirus (Kenaga 1979) 96hr, Pimephales promelas (Solon & Nair 1970)
Other information about water organisms	LOEC 3.16 mg/l, Colpidium campylum (Dive et al. 1980).	

1052 • Fenethcarb

30087-47-9

Synonyms	3,5-Diethylphenyl-n-methylcarbamate	
LC50 values to crustaceans, mg/l	1	24hr, Daphnia magna (Sanders & Cope 1966)
LC50 values to fishes, mg/l	35	96hr, Salmo gairdneri (Macek & McAllister 1970)

1053 • Fenitrothion

122-14-5

Synonyms	0,0-Dimethyl-0-(methyl-4-nitrophenyl)phosphorothioate 0,0-Dimethyl-0-(4-nitro-m-tolyl)phosphorothioate	
Use	Active ingredient in insecticides; acaricide.	
Molecular weight	277.25	
Vapour pressure, mmHg	0.000054 20 °C	
Water solubility, mg/l	30	
Melting point, °C	0.3	(MITI 1992)
Boiling point, °C	140–145	
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 20 mg/l (MITI 1992).	
Bioconcentration factor, fishes	200–250 8.0–53.6 1.5–101.7	 8w, Cyprinus carpio, conc 0.02 mg/l 8w, Cyprinus carpio, conc 0.002 mg/l (MITI 1992)
Bioconcentration factor, crustaceans	69	21d (Verschueren 1983)
Bioconcentration factor, algae	181	21d
LD50 values to mammals in oral exposure, mg/kg	250 142	orl-rat orl-cat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	750	skn-rat (Lewis & Sweet 1984)
LC50 values to mammals in inhalation exposure, mg/m³	378	4hr, ihl-rat (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	25 280 17.8–25.0 11 56.2 316 316	orl-bwd orl-ckn (Lewis & Sweet 1984) orl-Agelaius phoeniceus orl-Sturnus vulgaris orl-Coturnix coturnix orl-Passer domesticus orl-Carbodacus mexicanus (Schafer et al. 1983)
LD50 values to birds in dermal exposure, mg/kg	504	skn-dck (Lewis & Sweet 1984)

Effects on invertebrates	Isonychia sp.; LC50, 2d, 0.049 mg/l Ophiogomphus sp.; LC50, 2d, 0.045 mg/l Phasganophora sp.; LC50, 2d, 0.039 mg/l Pycnopsyche sp.; LC50, 2d, 0.137 mg/l Simulium venustum, LC50, 2d, 0.148 mg/l (Poirier & Surgeoner 1987).	
Effects on plants	Seeds of Betula alleghaniensis (yellow birch) and Betula paperifera (white birch) were exposed to the water-fenitrothion mix during stratification in the petri dishes. Seeds of both species showed reduced germination following exposure to 10 ppm fenitrothion (approximating a normal field dosage of 4 oz/acre (= 0.307 kg/ha) and marked toxicological damage when exposed to 1000 ppm fenitrothion. Weinberger et al. 1978	
EC50 values to algae, mg/l	1.2	rpd, act,24hr, Selenastrum capricornutum (Corture et al. 1982)
LC50 values to crustaceans, mg/l	0.0092	72hr, Daphnia magna (Verschueren 1983)
	12–55	96hr, Saccobranchus fossilis (Verma et al. 1982)
	0.05	Daphnia pulex (Hashimoto & Nishiuchi 1981)
	0.0061 0.0031 0.0014	1d, Macrobrachium lamarrei 2d, Macrobrachium lamarrei 3d, Macrobrachium lamarrei (Mary et al. 1986)
	0.269	2d, Orconectes propinquus (Poirier & Surgeoner 1987)
	0.0022	4d, Palaemon paucidens (Takimoto et al. 1987b)
EC50 values to crustaceans, mg/l	0.0016	1d, Daphnia pulex (Takimoto et al. 1987b)
LC50 values to fishes, mg/l	0.7 55 1.28 2.72 1.5 6 8.2 3.4 3.6	act, Salmo gairdneri (Kenaga 1979) 48hr, Channa punctata (Toor & Kaur 1974) 48hr, Salmo gairdneri (Verma et al. 1978) 48hr, Lepomis macrochirus (Verma et al. 1978) 24hr, Cyprinus carpio (Hashimoto et al. 1982) 48hr, Sarotheredon aureus (Koundinya & Ramamurthi 1982) 48hr, Cyprinus carpio (Hashimoto & Nishiuchi 1981) 48hr, Carassius auratus (Hashimoto & Nishiuchi 1981) 48hr, Oryzias latipes (MITI 1992)
Effects on the physiology of water organisms	Cyprinus carpio; 0.1 mg/100g/d,10d, biochemical effect (change in physiochemical process including glycogen uptake, cholesterol levels and lipid analysis) (Kobayashi et al. 1987).	
Other information about water organisms	Physa acuta; LC50, 4d, > 10 mg/l; Cipangopaludina japonica; LC50, 4d, > 10 mg/l (Takimoto et al. 1987a). Oryzias latipes; 0.0728 mg/l; 0.03d 0.0743 mg/l; 0.03d avoidance or attraction to a chemical gradient (Hidaka & Tatsukawa 1986). Procambarus clarkii; 0.2 mg/l, 4d, 100% mortality or 0% survival including algicidal and herbicidal effects (Andreu-Moliner et al. 1986).	

1054 • Fennosan H-30 * 148-24-3

Synonyms	8-Quinolinol	
Active ingredients	8-hydroxyquinolineacetate * 42%	
Use	Slimicide.	
LD50 values to birds in oral exposure, mg/kg	> 104	orl-Agelaius phoeniceus 8-quinolinol (Schafer et al. 1983)

LC50 values to crustaceans, mg/l	11.5	96hr, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	18	96hr, Alburnus alburnus (Linden et al. 1979)

1055 • Fennotox S 2 * 65280-29-7

Active ingredients	Ziram * 22.5%; Carbendazim * 2.5%	
Chemicals in the product	Ziram * 22.5%; Carbendazime * 2.5%	
Use	Pesticide.	
LC50 values to crustaceans, mg/l	0.4	96hr, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	3–4	96hr, Alburnus alburnus (Linden et al. 1979)

1056 • Fenpropanate 39515-41-8

LC50 values to fishes, mg/l	0.077 0.009	24hr, Salmo gairdneri 24hr, Salmo gairdneri (Coats & O'Donnell-Jefferey 1979)

EF

1057 • Fensulfothion 115-90-2

Synonyms	0,0-Diethyl-0-(4-(methylsulfinyl)-phenyl)-phosphorothioate	
Use	Insecticide.	
State and appearance	Yellowish oily liquid.	
Molecular weight	308.37	
Water solubility, mg/l	1600	
Boiling point, °C	138–141	
Total degradation in soil	Persistance in soil (10 ppm): 5% remaining 4 weeks incubation (nonsterile sandy loam) (Verschueren 1983).	
LD50 values to mammals in oral exposure, mg/kg	2	orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	3	skn-rat (Lewis & Sweet 1984)
LDLo values to mammals in oral exposure, mg/kg	9	orl-gpg (Lewis & Sweet 1984)
Other information about mammals	LDfr = 50.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).	
LD50 values to birds in oral exposure, mg/kg	0.237–0.316 0.562 1.78 0.316 0.422 0.562 0.237	orl-Agelaius phoenicus orl-Sturnus vulgaris orl-Coturnix coturnix orl-Passer domesticus orl-Quiscalus quiscula orl-Columba livia orl-Quelea quelea (Schafer et al. 1983)
LD50 values to birds in dermal exposure, mg/kg	3	skn-dck (Lewis & Sweet 1984)

1058 • Fenthion

55-38-9

Synonyms	0,0-Dimethyl-0-(3-methyl-4-methylthiophenyl)-phosphorothioate Baytex Phosphorothioic acid, 0,0-dimethyl-,0-(4-methylthio)-m-tolyl) ester Baycid Bayer 9007 Bayer 29493 m-Cresol, 4-(methylthio)-, 0-ester with 0,0-dimethylphosphorothioate 0,0-Dimethyl-0-4-(methylmercapto)-3-methylphenylthiophosphate 0,0-Dimethyl 0-(4-methylthio-3-methylphenyl)phosphorothioate 0,0-Dimethyl 0-(4-(methylthio)-m-tolyl)phosphorothioate DMTP Lebaycid Mercaptophos
Sumformula of the chemical	C10H15O3PS2
Products containing the chemical	Baytex * fenthion as effective agent
Use	Herbicide, insecticide.
Way to effect	Systemic and contact.
Molecular weight	278.34
Specific gravity (water=1)	1.25 at 20/4 C
Vapour pressure, mmHg	0.00003 20 °C
Water solubility, mg/l	55
Boiling point, °C	87
Total degradation in water	After 4 weeks 0% of original compound found (river water in a sealed glass jar (Verschueren 1983).
LD50 values to mammals in oral exposure, mg/kg	180 orl-rat 105 orl-mam (Lewis & Sweet 1984) 215–300 orl-rat (Martin 1968) 400 orl-gpg 118 orl-mus (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	50 unk-hmn 330 skn-rat (Lewis & Sweet 1984) 320–330 skn-rat (Martin 1968) 46 ims-domestic animal 46.2 ims-mam 200 ipr-mus 320 ivn-mus 98 skn-domestic animal 330 skn-rat (Sweet 1987)
LDLo values to mammals in non-oral exposure, mg/kg	310 ipr-gpg 260 ipr-rat (Sweet 1987)
LCLo values to mammals in inhalation exposure, mg/kg	1 ihl-gpg, 2hr ihl-mus, ihl-rat, ihl-rbt (Sweet 1987)

TDLo values to mammals in oral exposure, mg/kg	1050 orl-mus, multigenerations effects on fertility 1730 orl-mus, 103W-C, tumorigenic 257 orl-man (Sweet 1987)
TDLo values to mammals in non-oral exposure, mg/kg	40 ipr-mus, 11d preg. effects on embtyo or fetus (Sweet 1987)
Other information about mammals	ALD = 94.0 mg/kg, act, orl, deer mouse; LDfr = 62.5 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).
Carcinogenicity	NCI carcinogenesis bioassay completed: results negative, rat; results indefinite, mus (Lewis & Sweet 1984). NCI carcinogenesis bioassay (feed); clear evidence: mouse (Sweet 1987).
LD50 values to birds in oral exposure, mg/kg	1.7 orl-Agelaius phoeniceus (Schafer et al. 1983) 1.8 orl-bwd 1.8 orl-pgn (Lewis & Sweet 1984) 1.3 orl-wild bird 5.9 orl-dck 1.78 orl-pgn 11 orl-qal (Sweet 1987) 1.69–3.50 orl-Agelaius phoeniceus 5.30–17.8 orl-Sturnus vulgaris 17.8 orl-Coturnix coturnix 2.37–5.62 orl-Passer domesticus 4.22–7.50 orl-Quiscalus quiscalus 1.78 orl- Columba livia 13.3 orl-Carpodacus mexicanus 2.37 orl-Xanthocephalus xanthocephalus 1.00–1.33 orl-Falco sparverius 4.22–5.62 orl-Pica pica 7.5 orl-Molothrus ater 2.37 orl-Zenaida macroura 1.33 orl-Quelea quelea 5.62 orl-Turdus migratorius (Schafer et al. 1983)
LD50 values to birds in dermal exposure, mg/kg	44 skn-dck (Sweet 1987)
Effects on amphibia	LC50 (96hr) 0.00084 mg/l, tadpoles of Rana hexadactyla (Khangarot et al. 1985).
Effects on arthropods	LC50, 96hr, 0.0045 mg/l, Pteronarcys californica (Sanders & Cope 1968). Ricefield spider; Oedothorax insecticeps; LD50: 500 ppm (Ishikura 1972). Insect larvae (Chaoborus): LC50, 48hr: 0.008 ppm (Cloeon): LC50, 48hr: 0.012 ppm (Verschueren 1983).
EC50 values to algae, mg/l	3.33 rpd, act, Chlamydomonas reinhardii (Lee & Hong 1982)

LC50 values to crustaceans, mg/l	0.0008	48hr, Daphnia magna (Sanders & Cope 1966)
	0.0084	96hr, Gammarus lacustris (Sanders 1969)
	0.11	96hr, Gammarus fasciatus
	0.005	120hr, Palaemonetes kadiakensis
	0.0015	20d, Palaemonetes kadiakensis
	0.05	96hr, Orconectes nais
	1.8	96hr, Asellus brevicaudus (Sanders 1972)
	0.00092	48hr, Simocephalus serrulatus
	0.0008	48hr, Daphnia pulex (Sanders & Cope 1966)
	0.014	48hr, Gammarus pulex (Bluzat & Seuge 1979)
	0.006	act, Daphnia pulex (Nishiuchi & Hashimoto 1967)
	0.0008	act, Daphnia magna (Kenaga 1979)
LC50 values to fishes, mg/l	2.44	96hr, Pimephales promelas
	1.33	96hr, Salmo trutta
	1.32	96hr, Oncorhynchus kisutch
	1.65	96hr, Perca fluviatilis
	1.38	96hr, Lepomis macrochirus
	0.93	96hr, Salmo gairdneri (Macek & McAllister 1970)
	1.9	96hr, Carassius auratus
	2.5–3.3	96hr, Cyprinus carpio (Pesticide Manual 1983)
	1.88	act, Lepomis macrochirus
	0.93	act, Salmo gairdneri
	2.44	Pimephales promelas (Kenaga 1979)
	1.62	96hr, Cyprinus carpio (Kemp et al. 1973)
Other information about water organisms	EC (20hr), pht, 0.010 mg/l: Dunaliella euchlora Phaeodactylum tricornutum Skeletonema costatum Cyclotella nana (Walsh 1972).	
	LC50, 48hr, 6.4 mg/l, Lymnea stagnalis (Bluzat & Seuge 1979).	

1059 • Fentrifanil 62441-54-7

LC50 values to fishes, mg/l	0.009	96hr, Cyprinodon variegatus (Borthwick & Walsh 1981)

1060 • Fenuron 101-42-8

Synonyms	1,1-Dimethyl-3-phenylurea Phenyldimethylurea Funulon N-Phenyl-N,N-dimethylurea 3-Phenyl-1,1-dimethylurea
Sumformula of the chemical	C9H12N2O
Use	Herbicide. Weed and brush killer.
State and appearance	White, crystalline solid.

Vapour pressure, mmHg	0.00016 at 60 °C
Melting point, °C	132
Log soil sorption coefficient, log Kom	1.43 (Sabljic 1987)
Other physicochemical properties	Hydrolyses at high temperature or in acid or alkali. – Will be dissolved in water. As time passes more will be dissolved as aniline than as original species. Will dissolve slowly (Sax 1986). Sparingly soluble in hydrocarbon solvents, stable toward oxidation and moisture.
Other reactions in atmosphere	When heated to decomposition emits highly toxic fumes. Air pollution high (Sax 1986).
Total degradation in soil	Persistent in soil for 8 months (Sax 1986).
Total degradation in water	Not persistent over 2 weeks in river water (Sax 1986).
Other information about metabolism	Food chain contamination potential: negative (Sax 1986).
Other information about bioaccumulation	Potential for accumulation: Microorganisms effect de-alkylation. Negative (Sax 1986).
LD50 values to mammals in oral exposure, mg/kg	6400 orl-rat 7500 orl-rat (Sax 1986)
Mutagenicity	Suspected of affecting DNA. Potential (Sax 1986). Mutagen data: dni, mus, orl, 500 mg/kg (Sax 1986).
EC50 values to algae, mg/l	0.75 rpd, 10d, Chlorococcum sp. 0.75 rpd, 10d, Phaeodactylum tricornutum (Walsh 1972)
EC50 values to fishes, mg/l	53 96hr, Lepomis macrochirus (Sax 1986)
Other information about water organisms	1.0 mg/l, 24hr, Crangon crangon, 10% mortality; 1.0 mg/l, 48hr, Crangon crangon, 10% mortality; 2.9–29, marine plankton, lethal or no growth; 1 mg/l, 4hr, phytoplankton, 41% inhibition; > 10 mg/l, 48hr, hard clam eggs, LC50; > 5 mg/l, 288hr, hard clam larvae, LC50 (Sax 1986).

1061 • Fenvalerate 51630-58-1

Synonyms	Cyano-(3-phenoxyphenyl)methyl-4-chloro-α-(1-methylethyl)-benzeneacetate
Use	Pesticide, insecticide (pyretroid).
Molecular weight	419.93
Water solubility, mg/l	0.085 room temperature
LD50 values to mammals in oral exposure, mg/kg	451 orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	2500 skn-rbt (Lewis & Sweet 1984)
LC50 values to crustaceans, mg/l	0.00002 96hr, Mysidopsis bahia (Borthwick & Walsh 1981) 0.0019 96hr, Nitocra spinipes (Linden et al. 1979)

EC50 values to crustaceans, mg/l	0.00109 0.00021 0.00049 0.00016–0.00029 0.00180–0.00658 0.00083–0.00252 0.00025 0.00012	1d, mbt, Ceriodaphnia lacustris 2d, mbt, Ceriodaphnia lacustris 1d, mbt, Daphnia galeata mendotae 2d, mbt, Daphnia galeata mendotae 1d, mbt, Daphnia magna 2d, mbt, Daphnia magna 1d, mbt, Diaptomus oregonensis 2d, mbt, Diaptomus oregonensis (Day & Kaushik 1987)
LC50 values to fishes, mg/l	0.00015 0.0007 0.0001	96hr, Oncorhynchus kisutch 96hr, Ictalurus punctatus 96hr, Salmo gairdneri (Mauck & Olson 1976)
	0.00184	96hr, Fundulus heteroclitus (Trim 1987)
	0.005 0.002	96hr, Pimephales promelas 96hr, Salmo gairdneri (Holcombe et al. 1982)
	0.121 0.076 0.021	96hr, Cyprinodon variegatus (Borthwick & Walsh 1981) 24hr, Salmo gairdneri 30% EC, 24hr, Salmo gairdneri (Coats & O'Donnell-Jefferey 1979)
	0.002–0.003	96hr, Alburnus alburnus (Linden et al. 1979)
	0.00106–0.00169 0.00093–0.00113	1d Pimephales promelas 2d Pimephales promelas (Day & Kaushik 1987)
LOEC values to fishes, mg/l	0.00043	srv, schr, Pimephales promelas (Spehar et al. 1982)
NOEC values to fishes, mg/l	0.00033	srv, schr, Pimephales promelas (Spehar et al. 1982)
Effects on the physiology of water organisms	Salmo gairdneri; 0.006 mg/l, 0.25 d, hematological effect (change in various blood parameters such as red blood cell count, hematocrit, and serum osmolarity) (Natochin et al. 1987). Salmo gairdneri; 0.412 mg/l, 0.45d, 100% mortality or 0% surviving including algicidal and herbicidal effects (Bradbury et al. 1987).	

1062 • Ferbam 14484-64-1

Synonyms	Ferridimethyldithiocarbamate	
Use	Fungicide.	
Molecular weight	416.51	
LD50 values to mammals in oral exposure, mg/kg	4000 3400	orl-rat orl-mus (Lewis & Sweet 1984)
LDLo values to mammals in oral exposure, mg/kg	450	orl-gpg (Lewis & Sweet 1984)
EC50 values to microorganisms	0.2 10	15 min Microtox (Van Leeuwen et al. 1985) Nitrification (Van Leeuwen et al. 1985)
EC50 values to algae, mg/l	2.4	rpd,96hr, Chlorella pyrenoidosa (Leeuwen et al. 1985)
LC50 values to crustaceans, mg/l	0.09 0.18	48hr, Daphnia magna (Leeuwen et al. 1985) act, Daphnia pulex (Hashimoto & Nishiuchi 1981)

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LC50 values to fishes, mg/l	0.09 0.09 0.13	96hr, Poecilia reticulata (Leeuwen et al. 1985) 48hr, Cyprinus carpio (Hashimoto & Nishiuchi 1981) 48hr, Carassius auratus (Hashimoto & Nishiuchi 1981)

1063 • Ferric chloride 7705-08-0

Sumformula of the chemical	FeCl2	
Use	Used as a coagulant for sewage and industrial wastes, as an oxidizing and chlorinating agent, as a disinfectant, in copper etching and as a mordant.	
State and appearance	Brown crystals, soluble in water, alcohol and glycerol.	
Molecular weight	162.2	
Melting point, °C	300	
LD50 values to mammals in oral exposure, mg/kg	1278	orl-mus (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	68 142	ipr-mus (Lewis & Sweet 1984) ivn-mus (Lewis & Sweet 1984)
EC50 values to crustaceans, mg/l	183 124 160 120	2 days, Asellus aquaticus 4 days, Asellus aquaticus 2 days, Crangonyx pseudogracilis 4 days, Crangonyx pseudogracilis (Martin & Holdich 1986)

1064 • Ferrochromolignosulfonate 8075-74-9

LC50 values to fishes, mg/l	1500	96hr, Salmo gairdneri (Sprague & Logan 1979)

1065 • Ferrous sulfate 7720-78-7

EC50 values to crustaceans, mg/l	143 95	2d, mbt, Crangonyx pseudogracilis 4d, mbt, Crangonyx pseudogracilis (Martin & Holdich 1986)

1066 • Flamprop-isopropyl 57353-42-1

Use	Active ingredient in herbicides.	
LC50 values to fishes, mg/l	3.3	Salmo gairdneri (Pesticide Manual 1983)

1067 • Fluchloralin 33245-39-5

Synonyms	Basalin	
Use	Herbicide.	
Log soil sorption coefficient, log Kom	3.56	(Sabljic 1987)
Effects on plants	Vicia sativa (L.) was subjected to preemergence sprays of fluchloralin (2.5 kg/ha) → a significant decrease in mean leaf area (Prakash et al. 1978).	
Effects on the physiology of water organisms	Anacystis sp., < 300 mg/l, growth effect; 6hr, 100 mg/l, effect on nitrogen fixation. Nostoc muscorum, 25 mg/l, lethal effect; 8–20 mg/l, photosynthesis effect (Singh & Tiwari 1988).	

1068 • Fluoranthene 206-44-0

Sumformula of the chemical	C16H10	
Log octanol/water coefficient, log Pow	4.7 5.22 5.2	(Anon. 1986) observed (Chin et al. 1986) (Sangster 1989)
Effects on arthropods	LC50, 1 d: Aedes aegypti: 0.010 mg/l Aedes taeniorhynchus: 0.048 mg/l Culex quinquefasciatus: 0.045 mg/l (Borovsky et al. 1987).	
LC50 values to crustaceans, mg/l	320	48hr, Daphnia magna (LeBlanc 1980)
Other information about water organisms	Daphnia magna: lethal threshold concentration (LT50): 0.009 mg/l, 0.45d (Newsted & Giesy 1987).	

1069 • Fluorene 86-73-7

Synonyms	o-Biphenylenemethane 2,2'-Methylenebiphenyl	
Sumformula of the chemical	C13H10	
Water solubility, mg/l	< 100	(MITI 1992)
Melting point, °C	112–115	(MITI 1992)
Boiling point, °C	298	(MITI 1992)
Log octanol/water coefficient, log Pow	4.18 4.38 4.18	observed (Chin et al. 1986) (Mackay 1982) (Sangster 1989)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	396–821 219–830	8w, Cyprinus carpio, conc 0.02 mg/l 8w, Cyprinus carpio, conc 0.002 mg/l (MITI 1992)
LD50 values to birds in oral exposure, mg/kg	> 101	orl-Agelaius phoeniceus (Schafer et al. 1983)
EC50 values to algae, mg/l	15.5	rpd, act, Dunaliella bioculata (Heldal et al. 1984)
LC50 values to fishes, mg/l	5.15	48hr, Oryzias latipes (MITI 1992)

1070 • 9-Fluorenone 486-25-9

Sumformula of the chemical	C13H8O	
Log octanol/water coefficient, log Pow	3.58	(Sangster 1989)
LD50 values to birds in oral exposure, mg/kg	> 96.0	orl-Agelaius phoeniceus (Schafer et al. 1983)
EC50 values to algae, mg/l	5.7	grw, act, Dunaliella bioculata (Heldal et al. 1984)

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1071 • Fluorescent-260 16090-02-1

Sumformula of the chemical	C40H38N12O8S2.2Na
Water solubility, mg/l	5 (MITI 1992)
Melting point, °C	> 270 (MITI 1992)
Bioconcentration factor, fishes	1.4–4.7 6w, Cyprinus carpio, conc 0.2 mg/l < 6.4–28 6w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	50 48hr, Oryzias latipes (MITI 1992)

1072 • Fluorine and fluoride compounds 7782-41-4

Synonyms	Fluorides F2 (CAS 7782-41-4)
Sumformula of the chemical	F2
EINECS-number	2319548
Global release, kt/yr	16.3 atmosphere, 1969, USA, industrial (NAS 1971)
Use	In cement, glass and ceramic industry (fluorides). Phosphate fertilizers contain 1–4% fluorides.
Molecular weight	38
Other bindings	F- binds to minerals (CaCO3 and CaPO4) in sea water and the soluble forms are MgF+ (47%) and calcium and sodium fluorides (3%) (Miller & Kester 1976). In fresh water fluoride appears mostly in particular form bind to clay particles and detritus (Borg 1976). Fluorides bind strongly to clay particles in soil (Borg 1976).
Metabolism in mammals	Absorbtion from alimentary canal is very effective, which has been shown experimentally for example with rats. Approximately half of absorbed fluoride is stored in skeleton and dentine, the other half is excreted via urine (NAS 1974).
Other information about bioaccumulation	Fluorides concentrate mainly to skeleton of fish. Salmo gairdneri from rivers containing 12–14 mg/l: 2000 mg F-/kg in skeleton (Neuhold & Sigler 1960). Storing of fluorides has been observed also in muscular system of freshwater fishes and in roe (Neuhold & Sigler 1960). Clear accumulation of fluorides has been observed both in shell and solf parts of Mytilus even after short exposure times (20 and 96hr) (Wright & Davison 1975). Juveniles of oysters exposed to 50 mg/l F-: 40 x higher levels of F- (Nell & Livanos 1988).
Other information about mammals	Tolerance limits for chronic injuries in mammals: big, approximately 70 mg F/kg, dry weight in food (Eagers 1969).
Mutagenicity	Fluorides suspected genotoxic (Smith 1988).
Effects on amphibia	Frog roe, delayed devoloping, 1 mg F-/l (Groth 1975).

Effects on plants	< 0.0002 mg fluoride /m³ (0.00026 ppm) —no visible injury to conifers (Sidhu 1980). Batches of mature, non-senescent leaves of Poa annua were placed in cups containing fluoride solution (as Analar NAF) with about 10 mm of the base immersed in the solution. After 24 hours leaves were transferred to deion. Water —Poa developed a dull water-soaked appearance at the tips in concentrations of fluoride greater than 0.005 mg/ml. Eventually the leaf tips sediccated and necrosis spread towards the base (Davison et al. 1974). Certain plants have the ability to change the inorganic fluoride taken by the roots to organic fluorocompounds, above all to fluoroacetate, which is very toxic to mammals (Borg 1976). Lichens, visible injuries, yellow patches: 0.004 mg F/m³, 9 d (Gilbert 1973). Exposure of vegetation to lower fluoride concentration than those causing visible injuries inhibits photosynthesis, decreases growth and fertility and causes sterility of many species (Borg 1976). Conifers, inhibition of photosynthesis, 10 mg/kg, dry weight in needles; deciduous trees, inhibition of photosynthesis, 10–60 mg/kg, dry weight in leaves (McLaughlin & Barnes 1975).
EC50 values to algae, mg/l	2 F, EC63, 48hr, Chlorella (Groth 1975)
EC50 values to crustaceans, mg/l	98 48hr, mbt, Daphnia magna (Dave 1984)
LC50 values to fishes, mg/l	8.5 28d, sfd, Salmo gairdneri (Hebert & Shurben 1964) 2.3–7.3 Salmo gairdneri (Angelovic et al. 1961) 180–315 96hr, Pimephales promelas 200 96hr, Salmo gairdneri 340–460 96hr, Gasterosteus aculeatus (Smith et al. 1985) 2.7–4.7 20d, Salmo gairdneri (Neuhold & Sigler 1960) 2.6–6.0 10d, Salmo gairdneri (Angelovic et al. 1961) 75–95 20d, Cyprinus carpio (Neuhold & Digler 1960)
LOEC values to fishes, mg/l	13.6 schr, Pimephales promelas (McKim 1977)
NOEC values to fishes, mg/l	6.8 schr, Pimephales promelas (McKim 1977)
Other information about water organisms	Daphnia, disturbance in growth, reproduction, survival: approximately 4 mg F-/l (Dave 1984b). Salmo gairdneri, delayed hatching: 1.5 mg F-/l (Ellis et al. 1948).
Other information	Toxicity increases when water temperature increases (Angelovic et al. 1961). Decreased sensibility for fluorides in fish when water hardness increases (Neuhold & Sigler 1960). Fluorides have strong inhibitive effect on important enzymes through their ability to bild stabile complexes with metal ion activators of enzymes (e.g. Ca, Mg, Co, Mn) (Borg 1976).

1073 • 1-Fluoro-4-nitrobenzene 350-46-9

LC50 values to fishes, mg/l	28.4 96hr, Pimephales promelas (Veith et al. 1983)

1074 • Fluoroacetamide 640-19-7

Use	Rotenticide.	
LD50 values to birds in oral exposure, mg/kg	5.62 13.3	orl-Agelaius phoeniceus orl-Coturnix coturnix (Schafer et al. 1983)
LC50 values to crustaceans, mg/l	> 40	act, Daphnia pulex (Hashimoto & Nishiuchi 1981)
LC50 values to fishes, mg/l	> 40 > 40	48hr, Cyprinus carpio (Hashimoto & Nishiuchi 1981) 48hr, Carassius auratus (Hashimoto & Nishiuchi 1981)

1075 • 2-Fluorobutanamide-5-(2-(2,4-di-t-amylphenoxy)butanamide)phenol 346-10-1

Water solubility, mg/l	< 0.02	(MITI 1992)
Melting point, °C	158	(MITI 1992)
Total degradation in water	Biodegradation: 1% by BOD period: 28d substance: 100 mg/l sludge: 30mg/l (MITI 1992).	
Bioconcentration factor, fishes	0.3–1.9 < 1.7–5.0	6w, Cyprinus carpio, conc 2 mg/l 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 1000	48hr, Oryzias latipes (MITI 1992)

1076 • Fonophos 944-22-9

Synonyms	O-Ethyl-S-phenylethylphosphonodithioate	
Use	Insecticide.	
Molecular weight	246.34	
Half-life in soil, days	60	(Li et al. 1990)
Total degradation in soil	Persistance in soil (10 ppm): 5% remaining 20 weeks incubation (Verschueren 1983).	
LD50 values to mammals in oral exposure, mg/kg	3 1.3	orl-rat orl–rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	25 147	skn-rbt skn-rat (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	10 42.2 31.6 13.3 17.8 13.3	orl-Agelaius phoeniceus orl-Sturnus vulgaris orl-Coturnix coturnix orl-Passer domesticus orl-Quiscalus quiscula orl-Columba livia (Schafer et al. 1983)

LC50 values to fishes, mg/l	0.11 0.045	96hr, Salmo gairdneri 96hr, Lepomis macrochirus (Edwards 1977)
LOEC values to fishes, mg/l	0.033	srv, schr, Pimephales promelas (Pickering & Gilliam 1982)
NOEC values to fishes, mg/l	0.016	srv, schr, Pimephales promelas (Pickering & Gilliam 1982)

1077 • Formaldehyde

50-00-0

Synonyms	Methanal Methylaldehyde Formalin Formaline Formic aldehyde Methylene glycol Methylene oxide Oxymethylene Oxomethane	
Sumformula of the chemical	$CH2O$	
State and appearance	Colourless gas.	
Odour	Characteristic, hay, strawlike, pungent. USSR: human odour perception; non perception: 0.05 mg/m³; perception: 0.07 mg/m³; human reflex response; no response: 0.07 mg/m³; adverse response: 0.084 mg/m³. Odour index: 5000000 at 20 °C (Verschueren 1983).	
Molecular weight	30.03	
Specific gravity (water=1)	0.815	at -20/4 °C
Vapour density (air=1)	1.03	
Conversion factor, 1 ppm in air=	1.248	mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.815	ppm
Vapour pressure, mmHg	10 3883	-88 °C at 25 °C (Daubert & Danner 1985)
Melting point, °C	-118– -92	
Boiling point, °C	-21– -19	
Log octanol/water coefficient, log Pow	0.35 0.35	calc. (GEMS 1987) (Sangster 1989)
Henry's law constant, Pa x m^3/mol	0.033	(Dong & Dasgupta 1986)
Adsorption/desorption	Formaldehyde gas adsorbs somewhat to clay mineral at high concentrations of the gas, which is important to its use as a soil fumigant. (De & Chandra 1978)	
Other physicochemical properties	Very soluble, up to 55%. (Merck Index 1983)	

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Photochemical degradation in air	Formaldehyde absorbs UV radiation at wavelengths of 360 nm and so is capable of photolyzing in sunlight (Hampson 1980). The measured half-life for photolysis as measured in simulated sunlight is 6.0hr (Su et al. 1979). There are two photolytic channels; one producing H2 and CO and the H and CHO (Lowe et al. 1981). Based on its rate of reaction with photochemically produced hydoxyl radicals, formaldehyde will have a half-life of 19 hours in clean air and about half that long an polluted air. (Howard 1989). The hydroxy radical initiated oxidation of formaldehyde also occurs in cloud droplets to form formic acid, component of acid rain (Chameides & Davis 1983). When formaldehyde is irridiated in a reactor, the half-life is 50 min and 35 min in the absence and precence of NO2, respectively. The primary products formed are formic acid, HCl and CO (Howard 1989). Reaction with nitrate radicals, insignificant during the day, may be an important removal mechanism at night (USEPA 1982).
Other reactions in atmosphere	The hydroxy radical initiated oxidation of formaldehyde also occurs in cloud droplets to form formic acid, component of acid rain (Chameides & Davis 1983). When formaldehyde is irridiated in a reactor, the half-life is 50 min and 35 min in the absence and precence of NO2, respectively. The primary products formed are formic acid, HCl and CO (Howard 1989).
Photochemical degradation in water	In water, formaldehyde is hydrated and the hydrate does not have a chromophore that is capable of adsorbing sunlight and photolytically decomposing (Chameides & Davis 1983).
Other information about degradation	Biodegradation: + O2 → HCOOH → CO2 + H2O HCHO → CH3OH → CO2 + H2O + H2 Inhibition of anaerobic sludge digestion; at 100 mg/l; aerobic degradation; 135–175 mg/l (Verschueren 1983). Solutions containing formaldehyde are unstable, both oxidizing slowly to form formic acid and polymerizing (Kirk Othmer 1980). In the precence of air and moisture, polymerization readly takes place in concentrated solutions at room temperatures to form paraformaldehyde, a solid mixture of linear polyoxymethylene glycols cointaining 90–99% formaldehyde (USEPA 1984). In dilute aqueous solution formaldehyde exists almost exclusively as hydrated gem-diol (CH2(OH)2) (Dong & Dasgupta 1986). Formaldehyde in aqueous effluent is degraded by activated sludge and sewage in 48–72hr (Howard I 1989). In a die-away test using water from a stagnant lake, degradation was complete in 30hr under aerobic conditions and 48hr under anaerobic conditions (Kitchens et al. 1976).
Other information about bioaccumulation	Experiments performed on a variety of fish and shrimp show no bioconcentration of formaldehyde (Hose & Lightner 1980) (Sills & Allen 1979).
LD50 values to mammals in oral exposure, mg/kg	42 orl-mus (Lewis & Sweet 1984) 260 orl-gpg 800 orl-rat (Sweet 1987)

LD50 values to mammals in non-oral exposure, mg/kg	270	skn-rbt (Lewis & Sweet 1984)
	87	ivn-rat
	300	scu-mus
	420	scu-rat
	270	skn-rbt
		(Sweet 1987)
LC50 values to mammals in inhalation exposure, mg/m³	92	ihl-mam
	590	ihl-rat
		(Sweet 1987)
LDLo values to mammals in oral exposure, mg/kg	36	orl-wmn (Lewis & Sweet 1984)
	108	orl-wmn (Sweet 1987)
LDLo values to mammals in non-oral exposure, mg/kg	16	ipr-mus
	595	scu-dog
	240	scu-rbt
		(Sweet 1987)
LCLo values to mammals in inhalation exposure, mg/kg	820	ihl-cat, 8hr
	900	ihl-mus, 2hr
		(Sweet 1987)
TDLo values to mammals in oral exposure, mg/kg	200	orl-rat, 1d male, paternal effects (Sweet 1987)
TDLo values to mammals in non-oral exposure, mg/kg	259	ims-mus, 11d preg.
		effects on fertility
		effects on embryo or fetus
	240	ipr-mus, 7-14d preg.
		effects on embryo or fetus*
		specific developmental abnormalities
	500	ipr-mus, 5d male, paternal effects
	7	intratesticular-dog,1d male, paternal e.
	400	intratesticular-rat, 1d male
		effects on fertility
	46243	scu-rat, 20d male, paternal effects
	1170	scu-rat, tumorigenic
		(Sweet 1987)
TCLo values to mammals in inhalation exposure, mg/kg	1	ihl-rat, 24hr, 1-22d preg.
		effects on embryo of fetus
	0.035	ihl-rat, 8hr, 60d male, paternal eff.
	0.05	ihl-rat, 4hr, 1-19d preg.
		effects on newborn
	17	ihl-hmn, sense organs and special senses
		lungs, thorax or respiration
	0.3	ihl-man, sense organs and special senses behavioral
		(Sweet 1987)
TCLo values to mammals in inhalation exposure, ppm	8	ihl-hmn (Lewis & Sweet 1984)
	14.3	ihl-mus, rat, tumorigenic (Sweet 1987)
Other information about mammals	Skin and eye irritation data: skin, human, 0.150 mg, mild; eye, human, 1 ppm, 6 min nse, mild; skin, rabbit, 540 mg open, mild; eye, rabbit, 0.050 mg, 24hr, severe; eye, rabbit, 10 mg, severe (Sweet 1987).	

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<table>
<tr><td>Health effects</td><td>Man: severe toxic effects: 100 ppm = 120 mg/m³, 1min;
symptoms of illness; 30 ppm = 36 mg/m³;
unsatisfactory: 10 ppm = 12 mg/m³.
<table>
<tr><td>Conc. ppm</td><td>EXPOSURE TIME</td><td>EFFECTS</td></tr>
<tr><td>2–3</td><td></td><td>tingling of eyes, nose and throat;</td></tr>
<tr><td>4–5</td><td>10–30 min</td><td>irritation; discomfort;
lacrimation; some tolerance develops;
tolerable for some, not all;</td></tr>
<tr><td>20</td><td></td><td>short discomfort and lacrimation;</td></tr>
<tr><td>12</td><td></td><td>severe irritation;</td></tr>
<tr><td>13.8</td><td>30 min</td><td>nasal and eye irritation and lacrimation;</td></tr>
<tr><td>4</td><td>5 min</td><td>severe eye irritation;</td></tr>
<tr><td>1</td><td>5 min</td><td>8% of test panel reported eye irritation;</td></tr>
<tr><td>2</td><td>12 min</td><td>24% of test panel reported eye irritation;</td></tr>
<tr><td>4</td><td>5 min</td><td>100% of test panel reported eye irritation</td></tr>
<tr><td>2–4</td><td>5 min</td><td>33% of test panel reported eye irritation</td></tr>
<tr><td>0.9–1.6%</td><td>occup.
exposure</td><td>intense irritation;
itching of eyes; dry and sore throat;
increased thirst; disturbed sleep
(Verschueren 1983).</td></tr>
</table>
Eye irritation threshold: 3–10 ppm (Verschueren 1983).</td></tr>
<tr><td>Mutagenicity</td><td>Mutation data:
cyt, hmn, lym, 10 mg/l;
dnd, hmn, lug, 0.1 mmol/l;
DNA inhibition, esc, 5 mmol/l;
dnr, esc, 1.95 mg/l;
dns, hmn, hla, 10 nmol/l;
dlt, dmg, orl, 1300 ppm;
mrc, smc, 24 mmol/l;
microbial mutation without S9, microorganisms, 10 ppm;
mma, mus, lym, 25 mg/l;
otr, ham, kidney, 4 mg/l;
sin, dmg, orl, 250 ppm;
sce, ham, ovr, 0.110 mg/l;
sperm morphology, rat, orl, 200 mg/kg (Sweet 1987).</td></tr>
<tr><td>Effects on plants</td><td>305 kg formaldehyde (37%)/ha when applied to soil depressed growth of mycorrhizal sour orange (Citrus aurantium) seedlings. (Nemec 1980)</td></tr>
<tr><td>Maximum longterm immission concentration in air for plants, mg/m³</td><td>0.03 VDI 2306</td></tr>
<tr><td>Maximum longterm immission concentration in air for plants, ppm</td><td>0.02 VDI 2306</td></tr>
<tr><td>Effects on microorganisms</td><td>Bacteria: Escherichia coli, toxic, 1 mg/l (Verschueren 1983).
Toxicity threshold (cell multiplication inhibition test):
(formalin 35% w/w) bacteria (Pseudomonas putida): 14 mg/l (Bringmann & Kühn 1980a)</td></tr>
<tr><td>EC50 values to microorganism, mg/l</td><td>19 OECD 209 (Klecka et al. 1985)
11.6 INT (Dutton et al. 1986)</td></tr>
<tr><td>LOEC values to algae, mg/l</td><td>0.39 Microcystis aeruginosa (Bringmann & Kühn 1976)</td></tr>
<tr><td>LC50 values to fishes, mg/l</td><td>41 96hr, Branchydanio rerio
15–32.5 48hr, Leuciscus idus
(Wellens 1982)
84 96hr, Anquilla rostrata (Hinton & Eversole 1978)</td></tr>
</table>

Other information about water organisms	Ctenopharyngodon idella: LC50, 0.13 d, 160 ml/l; Cyprinus carpio: LC50, 0.13 d, 197 ml/l (Rosicky et al. 1986). Toxicity threshold (cell multiplication inhibition test) (35% w/w): bacteria (Pseudomonas putida): 14 mg/l algae (Microcystis aeruginosa): 0.39 mg/l green algae (Scenedesmus quadricauda): 2.5 mg/l protozoa (Entosiphon sulcatum): 22 mg/l protozoa (Uronema parduczi Chatton-Lwoff): 6.5 mg/l (Verschueren 1983) Scenedesmus, toxic, 0.3–0.5 mg/l; Daphnia toxic, 2 mg/l (Verschueren 1983). Toxicity threshold (cell multiplication inhibition test): (formalin 35% w/w) green algae (Scenedesmus quadricauda): 2.5 mg/l protozoa (Entosiphon sulcatum): 22 mg/l (Bringmann & Kühn 1980a)
Other effects on aquatic ecosystems	Reduction of amenities: taste and odour caused at 50 mg/l; osour threshold: average; 49.9 mg/l; range: 0.8–102 mg/l (Verschueren 1983).

1078 • Formaldehyde sodium bisulfate 1/2 hydrate

63148-74-3

Sumformula of the chemical	CH4O4 1/2SNa	
Water solubility, mg/l	> 100000	(MITI 1992)
Melting point, °C	91.0–91.5	(MITI 1992)
Boiling point, °C	198–200	(MITI 1992)
Total degradation in water	Biodegradation: 100–136% by BOD period: 28d substance:100 mg/l sludge: 30 mg/l (MITI 1992).	

1079 • Formamide

75-12-7

Synonyms	Methanamide	
Sumformula of the chemical	CH3NO	
Log octanol/water coefficient, log Pow	-1.51	(Sangster 1989)
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	

1080 • Formetanate-HCL

24353-61-5

Other information about mammals	ALD = 28 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987).

1081 • Formic acid 64-18-6

Synonyms	Aminic acid Formylic acid Hydrogen carboxylic acid Methanoic acid	
Sumformula of the chemical	CH_2O_2	
State and appearance	Colourless liquid.	
Odour	Pungent, penetrating. Odour index = 2200 at 20 °C (Verschueren 1983).	
Molecular weight	46.03	
Specific gravity (water=1)	1.22	at 20/4 °C
Vapour density (air=1)	1.6	
Conversion factor, 1 ppm in air=	1.91	mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.52	ppm
Vapour pressure, mmHg	35 54	20 °C 30 °C
Melting point, °C	8.4	
Boiling point, °C	101	
pKa	3.75 3.74	
Log octanol/water coefficient, log Pow	-0.54 -0.54	(Hansch & Leo 1979) (Sangster 1989)
Henry's law constant, Pa x m^3/mol	0.1121	calc. (Yaws et al. 1991)
LD50 values to mammals in oral exposure, mg/kg	4000 700 1100	orl-dog orl-mus orl-rat (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	940 145	ipr-mus ivn-mus (Sweet 1987)
LC50 values to mammals in inhalation exposure, mg/m^3	6200 15000	ihl-mus, 15min ihl-rat (Sweet 1987)
LDLo values to mammals in non-oral exposure, mg/kg	3000 239	ivn-dog ivn-rbt (Sweet 1987)
Other information about mammals	Skin and eye irritation data: skin, rabbit, 610 mg open, mild; eye, rabbit, 122 mg, severe (Sweet 1987).	
Mutagenicity	Mutation data: cyt, non-mammalian, cell types,, 100 mmol/l; microbial mutation without S9, esc, 70 ppm, 3hr; phage inhibition capacity, esc, 100 mmol/l; sin, dmg, ihl, 1000 ppm, 24hr; sin, dmg, ihl, 1000 ppm (Sweet 1987).	

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LD50 values to birds in oral exposure, mg/kg	> 111 orl-Agelaius phoeniceus (Schafer et al. 1983)
Effects on microorganisms	Slight inhibition of microbial growth after 24hr exposure at 5000 ppm (Verschueren 1983). Bacteria: Escherichia coli: no effect: 1 g/l.
Other information about water organisms	Algae: Scenedesmus, toxic, 100 mg/l; Arthropoda: Daphnia, toxic, 120 mg/l; Gammarus pulex, toxic, 2500 mg/l; Protozoa: Paramecium caudatum, toxic, 6000 mg/l; Vorticella campanula, toxic, 500 mg/l; Fish: Trutta iridea, perturbation level, 1000 mg/l (Verschueren 1983).

1082 • Formothion 2540-82-1

Use	Insecticide, acaricide.
LC50 values to crustaceans, mg/l	143 96hr, Saccobranchus fossilis (Verma et al. 1982)
LC50 values to fishes, mg/l	13 96hr, Heteropneustes fossilis (Singh & Srivastava 1982)

1083 • 1-Formyl-2-hydroxynaphthalene 708-06-5

Sumformula of the chemical	C11H802
Water solubility, mg/l	23.7 (MITI 1992)
Total degradation in water	Biodegradation: 29–102% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).

1084 • Fosalone 2310-17-0

LC50 values to crustaceans, mg/l	0.083 96hr, Saccobranchus fossilis (Verma et al. 1982)

1085 • Furan 110-00-9

Synonyms	1,4-Epoxy-1,3-butadiene
Sumformula of the chemical	C4H40
Water solubility, mg/l	96 (MITI 1992)
Melting point, °C	-85 (MITI 1992)
Boiling point, °C	32 (MITI 1992)
Log octanol/water coefficient, log Pow	1.34 (Sangster 1989)

EF

Total degradation in water	Biodegradation: 4% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	0.9–1.5 < 3.2–13	6w, Cyprinus carpio, conc 1 mg/l 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative. (Anon. 1987).	
LD50 values to birds in oral exposure, mg/kg	101	> 101, orl-Agelaius phoeniceus (Schafer et al. 1983)
LC50 values to fishes, mg/l	61 166	96hr, Pimephales promelas (Veith et al. 1983) 48hr, Oryzias latipes (MITI 1992)

1086 • Furazolidone 67-45-8

Effects on the physiology of water organisms	Cyprinus carpio; 0.1 mg/100g/day, biochemical effect (change in physiochemical process including glycogen uptake, cholesterol levels and lipid analysis) (Kobayashi et al. 1987).

EF

1087 • Furfural 98-01-1

Synonyms	Furfuraldehyde 2-Furaldehyde	
Sumformula of the chemical	C5H4O2	
Use	Solvent refining of lubricating oils, solvent for nitro cellulose, informedicate for tetrahydrofuran and furfuryl alcatrol.	
State and appearance	Colourless to yellowish liquid.	
Molecular weight	96.09	
Vapour pressure, mmHg	1	20 °C
Water solubility, mg/l	83000 83000 83000	20 °C 20 °C (Suntio et al. 1988) (MITI 1992)
Melting point, °C	-38.7 -36.5	(Suntio et al. 1988) (MITI 1992)
Boiling point, °C	150–155 (MITI 1992)	
Henry's law constant, Pa x m^3/mol	0.154	calc. (Suntio et al. 1988)
Total degradation in water	Biodegradation: 93.5% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	

LD50 values to mammals in oral exposure, mg/kg	127 400 50–100	orl-rat (Lewis & Sweet 1984) orl-mus (Lewis & Sweet 1984) orl-rat (Verschueren 1983)
LDLo values to mammals in non-oral exposure, mg/kg	620	skn-rbt (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	> 98	orl-Agelaius phoeniceus (Schafer et al. 1983)
Maximum longterm immission concentration in air for plants, mg/m³	0.08	VDI 2306
Maximum longterm immission concentration in air for plants, ppm	0.02	VDI 2306
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 16 mg/l (Bringmann & Kühn 1980a).	
LOEC values to algae, mg/l	2.7	Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to fishes, mg/l	32	96hr, Pimephales promelas (Vincent et al. 1976)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 31 mg/l protozoa (Entosiphon sulcatum): 0.6 mg/l (Bringmann & Kühn 1980a)	

1088 • Furfuryl alcohol

98-00-0

Water solubility, mg/l	> 100	(MITI 1992)
Melting point, °C	< -10	(MITI 1992)
Boiling point, °C	170	(MITI 1992)
Total degradation in water	Biodegradation: 75–79% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 180 mg/l (Bringmann & Kühn 1980a)	
LOEC values to algae, mg/l	5.2	rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 25 mg/l protozoa (Entosiphon sulcatum): 227 mg/l (Bringmann & Kühn 1980a)	

1089 • Furpyrinol

13411-16-0

Synonyms	6-(Hydroxymethyl)-2-(2-(5-nitro-2-furyl)vinyl)-pyridine	
Molecular weight	246.24	
LD50 values to mammals in oral exposure, mg/kg	4050 3720	orl-rat orl-mus (Lewis & Sweet 1984)

EF

LC50 values to fishes, mg/l	1.41 0.82 1 0.77 0.94	96hr, Salmo salar 96hr, Pimephales promelas 96hr, Salmo gairdneri (Marking et al. 1977) 96hr, Anguilla rostrata (Hinton & Eversole 1978) 96hr, Ictalurus punctatus (Mitchell & Plumb 1980)

1090 • Fyrol FR-2 — 13674-87-8

Synonyms	2-Propanol, 1,3-dichloro-, phosphate (3:1) Tris(1,3-dichloro-2-propyl)phosphate	
Sumformula of the chemical	C9H15Cl6O4P	
Water solubility, mg/l	110	(MITI 1992)
Melting point, °C	27	(MITI 1992)
Boiling point, °C	> 200	(MITI 1992)
Log octanol/water coefficient, log Pow	3.6–3.7	(MITI 1992)
Total degradation in water	Biodegradation: 0–4% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	0.30-3.3 < 2.2–22	6w, Cyprinus carpio, conc 0.02 mg/l 6w, Cyprinus carpio, conc 0.002 mg/l (MITI 1992)
LC50 values to fishes, mg/l	30 3.7	3hr, Carassius auratus (Ahrens et al. 1979) 48hr, Oryzias latipes (MITI 1992)

1091 • Gallium compounds — 7440-55-3

LC50 values to fishes, mg/l	3.51	28 d, Salmo gairdneri (Birge et al. 1980)

1092 • Garlon 3A — 57213-69-1

Synonyms	((3,5,6-Trichloro-2-pyridyl)oxy)acetic acid compound with N, N-diethylethanamine M 3724 Triclopyr triethylamine Triclopyr triethylamine salt	
Sumformula of the chemical	C7H4Cl3NO3.C6H15N	
Molecular weight	357.69	
LD50 values to mammals in oral exposure, mg/kg	2140	orl-rat (Sweet 1987)
LC50 values to crustaceans, mg/l	1170 1140	48hr, Daphnia magna 21d, Daphnia magna (Gersich et al. 1984)

LOEC values to crustaceans, mg/l	336	act, Daphnia magna (Gersich et al. 1984)
LC50 values to fishes, mg/l	316 267 498 463 353 311 472 275 457 420	1d, Oncorhynchus keta 4d, Oncorhynchus keta 1d, Oncorhynchus kisutch 4d, Oncorhynchus kisutch 1d, Oncorhynchus nerka 4d, Oncorhynchus nerka 1d, Oncorhynchus tshawytscha 4d, Oncorhynchus tshawytscha 1d, Salmo gairdneri 4d, Salmo gairdneri (Wan et al. 1987)

1093 • GC 4276

35944-86-6

Other information about mammals	LDfr = 25.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).	
LD50 values to birds in oral exposure, mg/kg	10 178	orl-Agelaius phoeniceus orl-Sturnus vulgaris (Schafer et al. 1983)

1094 • GC 6506

3254-63-5

Other information about mammals	LDfr = 50.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).	
LD50 values to birds in oral exposure, mg/kg	0.562 0.562	orl-Agelaius phoeniceus orl-Sturnus vulgaris (Schafer et al. 1983)

1095 • GD-174

19902-04-6

LC50 values to fishes, mg/l	0.05	96hr, Cyprinus carpio (Marking & Bills 1981)

1096 • Geraniol

106-24-1

Sumformula of the chemical	C10H18O	
EINECS-number	2033771	
Water solubility, mg/l	100	(MITI 1992)
Boiling point, °C	229–230	(MITI 1992)
Total degradation in water	Biodegradation: 36–70% by BOD (on the upward trend) period: 21d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

1097 • Germanium and germanium compounds

7440-56-4

LC50 values to fishes, mg/l	0.05	28 d, Salmo gairdneri (Birge et al. 1980)

1098 • Glucitol

50-70-4

Synonyms	D-Glucitol Sorbitol d-Sorbitol	
Sumformula of the chemical	C6H14O6	
Molecular weight	182.2	
LD50 values to mammals in oral exposure, mg/kg	17800 15900	orl-mus orl-rat (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	15000 9480 7100	ipr-mus ivn-mus ivn-rat (Sweet 1987)
TDLo values to mammals in oral exposure, mg/kg	1700	orl-wmn (Sweet 1987)

1099• Glycerin acetate

26446-35-5 *mono-
25395-31-7 *di-
102-76-1 *tri-

Water solubility, mg/l	> 100000	(MITI 1992)
Melting point, °C	< -10	(MITI 1992)
Boiling point, °C	272–273	(MITI 1992)
Total degradation in water	Biodegradation: 91–94% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

1100 • Glycerin-α-allylether

123-34-2

Synonyms	3-Propenoxy-1,2-propanediol	
Chemical oxygen demand, g 02/g	1.75	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.01	5 days (Bridie et al. 1979)
LC50 values to fishes, mg/l	> 5000	24hr, Carassius auratus (Bridie et al. 1979)

1101 • Glycerol

56-81-5

Synonyms	Glycerin Glycerine Glyceritol Glycyl alcohol 1,2,3-Propanetriol 1,2,3-Trihydroxypropane	
Sumformula of the chemical	C3H8O3	
Molecular weight	92.11	
Melting point, °C	20	(MITI 1992)
Chemical oxygen demand, g O2/g	1.16	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g O2/g	1	5 days (Bridie et al. 1979)
Total degradation in water	Biodegradation: 63% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	7750 4090 12600	orl-gpg orl-mus orl-rat (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	8982 8300 6199 5566 53 91 100	ipr-mus ipr-rat ivn-mus ivn-rat ivn-rbt scu-mus scu-rat (Sweet 1987)
TDLo values to mammals in oral exposure, mg/kg	1428	orl-hmn (Sweet 1987)
TDLo values to mammals in non-oral exposure, mg/kg	280 1600	intratesticular-rat, paternal effects intratesticular-rat, eff. on fertility (Sweet 1987)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): > 10000 mg/l (Bringmann & Kühn 1980a).	
LOEC values to algae, mg/l	2900	rpd, schr, Microcystis aeruginosa (Bringmann & Kuhn 1976)
LC50 values to fishes, mg/l	> 5000	24hr, Carassius auratus (Bridie et al. 1979)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): > 10000 mg/l protozoa (Entosiphon sulcatum): 3200 mg/l (Bringmann & Kühn 1980a).	

GHI

1102 • Glycidyl methacrylate 106-91-2

Sumformula of the chemical	C7H10O3
EINECS-number	2034419
Melting point, °C	< -10 (MITI 1992)
Boiling point, °C	196.8–197.9 (760 mmHg) (MITI 1992)
Total degradation in water	Biodegradation: 93–94% by BOD period: 28d substance: 100 mg/l sludge:30 mg/l (MITI 1992).

1103 • Glycidyltrimethyl ammonium chloride 3033-77-0

Synonyms	2,3-Epoxypropyltrimethyl ammonium chloride	
Chemical oxygen demand, g O2/g	0.53	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g O2/g	0	5 days (Bridie et al. 1979)
LC50 values to fishes, mg/l	5000	24hr, Carassius auratus (Bridie et al. 1979)

1104 • Glyoxal 107-22-2

Melting point, °C	15	(MITI 1992)
Boiling point, °C	51	(MITI 1992)
Total degradation in water	Biodegradation: 65% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LC50 values to fishes, mg/l	550 215	24hr, Pimephales promelas 96hr, Pimephales promelas (Conway et al. 1983)

1105 • Glyphosate 1071-83-6

Synonyms	N-(Phosphonomethyl)glycine	
Sumformula of the chemical	C3H8NO5P	
Use	Active ingredient in herbicides.	
Molecular weight	169.09	
Vapour pressure, mmHg	0.000000075, 25 °C (KEMI 1990)	
Water solubility, mg/l	12000	at 25 °C (KEMI 1990)

pKa	2.3 5.6 10.3	pKa1 pKa2 pKa3 (KEMI 1990)
Log octanol/water coefficient, log Pow	-3	(KEMI 1990)
Adsorption/desorption	Glyphosate was bound tightly to soil. Adsorption depends on concentration of unbound unorganic phosphorous. The higher is concetration the worse adsorption. (KEMI 1990)	
Mobility	The leaching of glyphosate was low on the study of soil thin-layer plates. The degradation product aminomethylphosphoric acid has more mobile than glyphosate. Koc: 300–11 000, Rf: 0.04–0.2 (KEMI 1990).	
Other physicochemical properties	Decomposes at 200 °C. (KEMI 1990)	
Photochemical degradation in soil	Photolysis half-life of glyphosate was about 3–4 weeks and little longer for the degradation product, aminomethylphosphoric acid (AMPA). (KEMI 1990)	
Hydrolysis in water	Glyphosate is relative stable in hydrolysis but degradationproduct aminomethylphosphoric acid is hydrolysed quicly. (KEMI 1990)	
Total degradation in soil	Degradation of glyphosate in soil is most part microbiprocess. The half-life varies from couple days to several years depending on the microbiactivity in soil. Degradation of degradationproduct aminomethylphosphoric acid is more slowly. (KEMI 1990)	
Total degradation in water	Degradation is quickliest in water where is high microbiactivity and low pH. The half-life is 7 weeks at pH 4.2. (KEMI 1990)	
Degradation and transformation products	Aminomethylphosphoric acid (AMPA) * major degradationproduct (KEMI 1990)	
LD50 values to mammals in oral exposure, mg/kg	470 1568 3800–4320	orl-rat orl-mus (Lewis & Sweet 1984) orl-rbt, orl-rat (KEMI 1990)
LD50 values to mammals in non-oral exposure, mg/kg	> 5000	idr-rbt (KEMI 1990)
LC50 values to mammals in inhalation exposure, mg/m³	8000	> 8 mg/l, ihl-rat (KEMI 1990)
Effects on bees	LD50 (48hr): > 100 µg/bee. (KEMI 1990)	
Effects on plants	13-day-old common cocklebur (Xanthium pensylvaticum) plants were treated with 15 µg glyphosate applied as droplets to the lowermost tru leaves —growth was inhibited rapidly following treatment; transport of P from roots to the aerial tissues was severely inhibited. (Nafzigen & Slife 1983)	
EC50 values to algae, mg/l	1.3 1.2	96hr, Skeletonema costatum (Anon. 1984) 96hr, Skeletonema costatum (KEMI 1990)
LC50 values to crustaceans, mg/l	780 5.3 3	48hr, Daphnia magna (Anon. 1984) 48hr, Daphnia magna (roundup) (Anon. 1984) 48hr, water flea (roundup) (Folmar et al. 1979)
EC50 values to crustaceans, mg/l	780	24hr, Daphnia magna (KEMI 1990)

LC50 values to fishes, mg/l	52–55	96hr, Salmo gairdneri (Hildebrand et al. 1982)
	15	96hr, Ctenopharyngodon idella (Tooby et al. 1980)
	140–220	96hr, Lepomis macrochirus
	97	96hr, Pimephales promelas
	130	96hr, Ictalurus punctatus
	140	24hr, technical glyphosate, S. gairdneri
	2.1	24hr, surfactant, S. gairdneri
	140–240	96hr, Salmo gairdneri (Folmar 1979)
	86	96hr, Salmo gairdneri
	120	96hr, Lepomis macrochirus
	168	96hr, Rasbora heteromorpha (Anon. 1984)
Other information about water organisms	NOEL, 21d, rpd, 50 mg/l, Daphnia magna. (KEMI 1990) LC50, 24hr, 38–140 mg/l, fish. (KEMI 1990) EC50, 24hr, mbt, 55 mg/l, mosquito larvae. LC50, 96hr, 281–934 mg/l, crayfish. (KEMI 1990)	

1106 • Glyphosate, isopropylaminesalt 38641-94-0

LC50 values to crustaceans, mg/l	930	48hr, Daphnia magna (Anon. 1984) (Monsanto)
LC50 values to fishes, mg/l	> 1000	96hr, Salmo gairdneri (Anon. 1984)

GHI

1107 • Gold and gold compounds 7440-57-5

Molecular weight	196.97	
LC50 values to crustaceans, mg/l	1.05	21d, Daphnia magna (Biesinger & Christensen 1972)
EC50 values to crustaceans, mg/l	0.18	21d, rpd, Daphnia magna (Biesinger & Christensen 1972)
LOEC values to crustaceans, mg/l	0.06	21d, rpd, Daphnia magna (Biesinger & Christensen 1972)

1108 • Gophacide 4104-14-7

Other information about mammals	ALD = 18.0 mg/kg, act, orl, deer mouse; LDfr = 74.1 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).	
LD50 values to birds in oral exposure, mg/kg	4.22–4.46	orl-Agelaius phoeniceus
	17.8	orl-Sturnus vulgaris
	15.9	orl-Columba livia (Schafer et al. 1983)

1109 • GS 14259 33693-04-8

Synonyms	2-(tert-Butylamino)-4-(ethylamino)-6-methoxy-s-triazine
Use	Herbicide.

Effects on plants	Soil was amended to give 2.0 ppm by weight of soil of GS 14259 —atrazine-susceptible lamb's-quarters (Chenopodium album L.) were killed soon after germination and emergence (Jensen et al. 1977).

1110 • Guaiacol

90-05-1

Synonyms	2-Methoxyphenol	
Water solubility, mg/l	26	(MITI 1992)
Melting point, °C	26–29	(MITI 1992)
Boiling point, °C	205	(MITI 1992)
Total degradation in water	Biodegradation: 88–91% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
LC50 values to fishes, mg/l	44	96hr, Salmo gairdneri (Voss et al. 1980)

1111 • Guazatine acetates

115044-19-4

Use	Fungicide.	
Water solubility, mg/l	> 3 000 000	(Pesticide Manual 1994)
Degradation point, °C	150	about 150 °C (Pesticide Manual 1994)
LD50 values to mammals in oral exposure, mg/kg	300	about 300 mg/guazatine acetates/kg (Pesticide Manual 1994)
LD50 values to birds in oral exposure, mg/kg	> 100	39202-39-6 Agelaius phoeniceus (Schafer et al. 1983)
Other information	Guazatine is produced by the amidination of technical iminodi(octamethylene)diamine, commercial guazatine contains numerous guanidines, in which the amino and imino groups of the polyamine chain form part, and polyamines; many of these bases are fungicidal (Pesticide Manual 1994).	

1112 • Halowax

51569-12-1

LC50 values to crustaceans, mg/l	0.44 0.074 0.069	halowax 1000, 96hr, Palaemonetes pugio halowax 1013, 96hr, Palaemonetes pugio halowax 1099, 96hr, Palemonetes pugio (Green & Neff 1977)

1113 • Heptachlor

76-44-8

Synonyms	1,4,5,6,7,8,8-Heptachlor-3a,4,7,7a-tetrahydro-4,7-endo-methano-indene	
Products containing the chemical	Drinox Heptamul Velsicol 104	
Use	Insecticide.	
Molecular weight	373.3	
Vapour pressure, mmHg	0.0003	25 °C

GHI

Water solubility, mg/l	34300 (MITI 1992)
Melting point, °C	95–96 (MITI 1992)
Log octanol/water coefficient, log Pow	5.44 (Anon. 1988) 5.44 (Mackay 1982) 6.13 (MITI 1992)
Henry's law constant, Pa x m³/mol	500 (Anon. 1988)
Mobility	Equilibrium distribution: *mass%* air 79.90 water 0.46 solid 19.64 (Anon. 1988).
Half-life in soil, days	2000 (Li et al. 1990)
Total degradation in soil	75–100% disappearance from soils: 2–5 years (Verschueren 1983).
Total degradation in water	0% of original compound found after 2 weeks in river water (initial concentration 10 µg/l) (Verschueren 1983). Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	300–21300 (Verschueren 1983) 2520–17300 10w, Cyprinus carpio, conc 0.001 mg/l 2020–15600 10w, Cyprinus carpio, conc 0.0001 mg/l (MITI 1992)
Bioconcentration factor, mollusca	250–17600 (Verschueren 1983)
Bioconcentration factor, crustaceans	200–8500 (Verschueren 1983)
LD50 values to mammals in oral exposure, mg/kg	40 orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	119 skn-rat (Lewis & Sweet 1984) 90 ukn-rat (Virtanen & Nuuja 1987)
Carcinogenicity	NCI carcinogenesis bioassay completed: results positive, mus; results negative, rat (Lewis & Sweet 1984).
LD50 values to birds in oral exposure, mg/kg	62 orl-ckn (Lewis & Sweet 1984)
Effects on arthropods	LC50, > 2,5 mg/l, 48hr, renewal, Tanytarsys dissimilis (Holcombe et al. 1983).
LC50 values to crustaceans, mg/l	0.0924 96hr, Saccobranchus fossilis (Verma et al. 1982) 0.052 Daphnia pulex (Frear et al. 1967) 0.404 96hr, Daphnia pulex (Podowski et al. 1979) 0.052 48hr, Daphnia magna (Frear & Boyd 1967) 0.058 act, Daphnia magna (Kenaga 1979) 0.0018 96hr, Palaemonetes kadiakensis (Sanders 1972)
EC50 values to crustaceans, mg/l	0.042 srv, 48hr, Daphnia pulex (Sanders & Cope 1966) 0.047 srv, 48hr, Simocephalus serrulatus (Sanders & Cope 1966)
NOEC values to crustaceans, mg/l	0.015 rpd, schr, Daphnia magna (Macek et al. 1976c)

LC50 values to fishes, mg/l	0.008	act, Salmo gairdneri (Kenaga 1979)
	0.00085	96hr, Leistomus canthurus (Schimmel et al. 1976)
	0.019	96hr, Salmo gairdneri (Katz 1961)
	0.017	96hr, Oncorhynchus tschawytscha (Verschueren 1983)
	0.064	96hr, Lepomis macrochirus (Podowski et al. 1979)
	0.185	96hr, Carassius auratus (Podowski et al. 1979)
	0.019	Lepomis macrochirus (Kenaga 1979)
	0.056	Pimephales promelas (Kenaga 1979)
	14.4	48hr, Oryzias latipes (MITI 1992)
LOEC values to fishes, mg/l	0.0018	srv, chr, Pimephales promelas (Macek et al. 1976c)
	0.0028	srv, schr, Cyprinodon variegatus (Ward & Parrish 1980)
NOEC values to fishes, mg/l	0.0009	srv, chr, Pimephales promelas (Macek et al. 1976c)
Effects on the physiology of water organisms	Tilapia mossambica; 0.030 mg/l, 5 d, histological effect (presence of physical damage to tissues) (Radhiah et al. 1986).	
Other information about water organisms	LC50, 1.45 mg/l, 96hr, renewal, Aplexa hypnorum (Holcombe et al. 1983).	

1114 • Heptachlor epoxide 1024-57-3

Log octanol/water coefficient, log Pow	5.4	(Mackay 1982)
Other information about mammals	Lethal dose in the brains of the bat is 3.4 mg/kg (Virtanen & Nuuja 1987).	
LC50 values to crustaceans, mg/l	0.00004	96hr, Penaeus duorarum (Schimmel et al. 1976)

1115 • Heptachloronorbornene 28680-45-7

Log octanol/water coefficient, log Pow	5.28	(Mackay 1982)
LC50 values to fishes, mg/l	0.086	96hr, Pimephales promelas
	0.06	30 d, Pimephales promelas (Spehar et al. 1979)

1116 • 4-(Heptaloxy)phenol 13037-86-0

Other information about water organisms	EC50, grw, 2 d, Tetrahymena pyriformis, 1.93 mg/l (Schultz 1987).

1117 • 2,2,4,4,6,8,8-Heptamethylnonane 4390-04-9

Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100.0 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).

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Bioconcentration factor, fishes	4.7–23.7 8w, Cyprinus carpio, conc 2 mg/l 12.6–176 8w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	1600 48hr, Oryzias latipes (MITI 1992)

1118 • Heptane

142-82-5

Use	Solvent.
Water solubility, mg/l	< 100
Boiling point, °C	98.4
Henry's law constant, Pa x m³/mol	273500 calc. (Yaws et al. 1991)
Volatilization	Relative volatility (nBuAc=1) = 3.62
TCLo values to mammals in inhalation exposure, ppm	1000 6 min., CNS-eff., rat

1119 • 1-Heptanol

111-70-6

Synonyms	n-Heptanol
Sumformula of the chemical	C7H16O
Log octanol/water coefficient, log Pow	2.62 (Sangster 1989)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 67 mg/l (Bringmann & Kühn 1980a).
EC50 values to microorganism, mg/l	918 Biodegradation inhibition (Vaishnav 1986) 9.9 15 min Microtox (Hermens et al. 1985)
LOEC values to algae, mg/l	3.5 rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
NOEC values to algae, mg/l	35 rpd, schr, Selenastrum capricornutum (Slooff et al. 1983)
LC50 values to crustaceans, mg/l	210 96hr, Nitocra spinipes (Linden et al. 1979) 70 48hr, Daphnia magna 49 48hr, Daphnia pulex 84 48hr, Daphnia cucullata (Canton & Adema 1978) 70 48hr, Asellus aquaticus (Slooff 1983) 60 48hr, Gammarus pulex (Slooff 1983)
LC50 values to fishes, mg/l	63 96hr, Branchydanio rerio 29–41 48hr, Leuciscus idus (Wellens 1982) 42–49 96hr, Alburnus alburnus (Linden et al. 1979) 43 48hr, Salmo gairdneri (Slooff et al. 1983) 38 96hr, Pimephales promelas (Broderius & Kahl 1985)

Other information about water organisms	LC50, 48hr, 26 mg/l, Tubificidae LC50, 48hr, 80 mg/l, Chironomus gr. thummi LC50, 48hr, 130 mg/l, Erpobdella octoculata LC50, 48hr, 40 mg/l, Lymnaea stagnalis LC50, 48hr, 200 mg/l, Dugesia cf. lugubris LC50, 48hr, 160 mg/l, Hydra oligactis LC50, 48hr, 160 mg/l, Corixa punctata LC50, 48hr, 109 mg/l, Ischura elegans LC50, 48hr, 36 mg/l, Nemoura cinerea LC50, 48hr, 134 mg/l, Cloeon dipterum (Slooff 1983) Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 17 mg/l protozoa (Entosiphon sulcatum): 31 mg/l (Bringmann & Kühn 1980a)

1120 • 2-Heptanone — 110-43-0

Synonyms	Methyl amyl ketone
Sumformula of the chemical	C7H14O
Use	Solvent.
Boiling point, °C	151.5
Log octanol/water coefficient, log Pow	1.98 (Sangster 1989)
LD50 values to mammals in oral exposure, mg/kg	1670 orl-rat

1121 • 3-Heptanone — 106-35-4

Synonyms	Ethyl butyl ketone
Use	Solvent.
Water solubility, mg/l	14300 20 °C
Boiling point, °C	147
Volatilization	Relative volatility (nBuAc=1) = 0.45
LD50 values to mammals in oral exposure, mg/kg	2760 orl-rat

1122 • 1-Heptene — 592-76-7

Log octanol/water coefficient, log Pow	3.99 (Sangster 1989)
Henry's law constant, Pa x m³/mol	40590 calc. (Yaws et al. 1991)

1123 • Hercules 22234 — 38727-55-8

Synonyms	Ethyl N-chloroacetyl-N-(2,6-diethylphenyl) aminoacetate
Effects on plants	Hercules 22234 reduced germination of dodder (Cuscuta australis) seeds by 37% at a concentration of 10 µg/ml (seeds were placed to Petri dishes on filter paper where the herbicide solution was added) (Giannopolitis 1979).

1124 • Hexabromo diphenyl ether 36483-60-0

Water solubility, mg/l	< 0.001 (MITI 1992)
Melting point, °C	148–151 (MITI 1992)
Log octanol/water coefficient, log Pow	> 6 (MITI 1992)
Total degradation in water	Biodegradation: 15% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	216–1310 8w, Cyprinus carpio, conc 0.01 mg/l 527–1490 8w, Cyprinus carpio, conc 0.001 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be accumulated on a medium level (Anon. 1987).
LC50 values to fishes, mg/l	> 500 48hr, Oryzias latipes (MITI 1992)

1125 • Hexabromobenzene 87-82-1

Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).

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1126 • Hexachlorobenzene 118-74-1

Sumformula of the chemical	C6Cl6
Products containing the chemical	Anticarie Bunt-Cure
Use	Fungicide; manufacturing pentachlorophenol; wood preservative; organic synthesis; impregnation of paper. Byproduct; intermediate.
State and appearance	White crystalline solid.
Molecular weight	284.76
Specific gravity (water=1)	2.044
Density, kg/m³	2075 24 °C
Vapour pressure, mmHg	0.0000109
Water solubility, mg/l	0.0032 20 °C 0.005 25 °C (Anon. 1986b)
Melting point, °C	230 (Suntio et al. 1988) 231 (MITI 1992)
Boiling point, °C	322 (Anon. 1986b) 330 (Anon. 1989)
Flashing point, °C	242

Log octanol/water coefficient, log Pow	4.13–7.42 (Sabljic 1987) 6.18 observed (Chin et al. 1986) 6.18 (Anon. 1988) 6.06 (Schwarzenbach et al. 1983) 4.13 (Hansch & Leo 1979) 5.5 (Chiou et al. 1982) 6.53 Yalkowsky et al.1979 5 (Konemann et al. 1979) 6.44 (Konemann et al. 1979) 5.4 (Wateral et al. 1982) 5.47 (Miller et al. 1984) 5.23 (Mackay 1982)
Henry's law constant, Pa x m³/mol	76 (Anon. 1988) 134 exptl. (Atlas et al. 1982) 139.8 25 °C (Anon. 1989)
Volatilization	The predicted evaporation rate from water in 0.08 in minute representing a half-life of approximately 8 hours from a 1-m-deep water column (Sax 1986).
Mobility	Equilibrium distribution: *mass%* air 10.11 water 0.39 solid 89.50 (Anon. 1988). Theoretical distribution: approximately 50% air approximately 40% water and sediment < 10% soil (Nordic 1988).
Other reactions in atmosphere	Air pollution: high. Hexachlorobenzene is disseminated in the air as dust particles and as a result of volatilization from sites having a high hexachlorobenzene concentration. Airborne, hexachlorobenzene-laden dust particles appear to have been a major factor in producing the blood levels in the general public, living near an industrial site in Louisiana (Sax 1986).
Photochemical degradation in water	Direct photolysis is not expected to be an important fate process for hexachlorobenzene in the aquatic environment although its photolysis in the presence of sensitizers has not yet been studied (Sax 1986).
Hydrolysis in water	No hydrolysis (Klöpffer 1978). Hydrolysis is not an expected fate (Sax 1986).
Half-life in soil, days	724 (Dawson et al. 1980) 1460 (Sax 1986)
Half-life in water, days	0.3–3 days, in river water 30–300 days, in lake and ground waters (Sax 1986)
Aerobic degradation in water	Not easily biodegradable in aerobic water environment (Tabak et al. 1981).
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).

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Other information about degradation	Degradation by Pseudomonas (200 mg/l, 30 °C): parent: 0% ring disruption in 120hr mutant: 0% ring disruption in 120hr (Verschueren 1983). Degradation of HEXACHLOROBENZENE:

ENVIRONMENT	*INIT.CONC. mg/l*	*REDOX-COND.*	*TEMP. °C*	*DEGRADATION %/day*	*REF.*
water	200	aerobic	30	0/120	a
water	5	aerobic	25	56/7	b
water	10	aerobic	25	21/7	b
water (adapted)	5	aerobic	25	5/7	b
water (adapted)	10	aerobic	25	0/7	b
soil	5.6	aerobic	-	0/570	c

a) Verschueren 1983
b) Tabak et al. 1981
c) Beall 1976
(Anon. 1987b).

Degradation in active sludge is significant (Anon. 1987b).

Very slow decreasing dechlorination (Åkermark et al. 1976).

Photochemical degradation: 14% in 24 hours (Klöpffer 1978).

Degradation products of special interest: pentachlorophenol, tetrachlorophenol (Anon. 1989).

Very persistent in soils, sediments, and aquatic systems (Sax 1986).

Metabolism in mammals	In nursing infant rhesus monkeys, hexachlorobenzene was concentrated mostly in body fat (1687 ppm), bone marrow (1526 ppm), lymph nodes (584 ppm), and adrenals (383 ppm), being 2 to 5.5 times higher in the infants' tissues than in the mothers' except for the thymus (Sax 1986).
Bioconcentration factor, fishes	1160–7762 (Verschueren 1983) 290000 Poecilia reticulata 21300 28d, Branchydanio rerio 4870–11390 14d, Branchydanio rerio (Anon. 1986b) 7900–18500 fish (Neely et al. 1974, Veith et al. 1979) 22000 Pimephales (Carlson & Kosian 1987) 287–15850 Gambusia affinis, Ictalurus punctatus fingerlings (Sax 1986) 23391 32d, Pimephales promelas (USEPA 1984) 11000–27000 8w, Cyprinus carpio, conc 0.0005 mg/l 6000–30000 8w, Cyprinus carpio, conc 0.00005 mg/ (MITI 1992)
Bioconcentration factor, mollusca	1360–3320 (Verschueren 1983)
Bioconcentration factor, crustaceans	770–1030 (Verschueren 1983) 200–1129 Daphnia magna (Sax 1986)
Bioconcentration factor, algae	320–1570 (Verschueren 1983) 24800 algae, 24hr (Freitag et al. 1982) 610–3969 Dedogonium cardiacum (Sax 1986)
Bioconcentration factor, other organisms	50000 bacteria (Verschueren 1983) 1248–2672 snails,Helisoma, Physa sp. (Sax 1986) 143–2622 Culex quinquifascistus (Sax 1986)
Other information about bioaccumulation	Confirmed to be accumulated on a high level (Anon. 1987).

LD50 values to mammals in oral exposure, mg/kg	10000 4000 1700	orl-rat orl-mus orl-cat (Lewis & Sweet 1984)
	1250	orl-whiterat (Verschueren 1983)
	10000 3500 1000 4000 1000 1700	orl-rat orl-rat orl-harbour porpoise orl-mus orl-rbt orl-cat (Anon. 1986b)
TDLo values to mammals in oral exposure, mg/kg	40 1000 1050 6972 1000	orl-rat, 10-13d preg, teratogenic effect orl-mus, 7-16d preg, teratogenic effect orl-rat, 30W-C, tumorigenic effect orl-mus, 83W-C, tumorigenic effect orl-ham, 18W-C, tumorigenic effect (Sax 1986)
Other information about mammals	Lethal dose in food to mink (Mustela vison) and ferret (Mustela putorius furo) was 125 mg/kg. < 25 mg/kg was disadvantageous to reproduction (Virtanen & Nuuja 1987).	
Health effects	During the period 1955–1960, few infants of Turkish mothers survived because of the consumption (by the mothers) of hexachlorobenzene-contaminated bread from which the fatal disorder pembe yara developed. – Irritation to the skin is possible. Also there have been reports of cutaneous porphyria among children in Turkey contaminated through the consumption of affected bread (Sax 1986). Chlorinated benzenes are irritating to the skin, conjunctivis, and mucous membranes of the upper respiratory tract. Prolonged or repeated contact with liquid chlorinated benzenes may cause skin burns. – Acute exposure to chlorinated benzenes may cause drowsiness, incoordination, and unconsciousness. – Chronic exposure may result in liver, kidney, and lung damage as indicated by animal experiments (Sax 1986).	
Carcinogenicity	Carcinogen to mice and hamsters (IARC 1979). Hexachlorobenzene was tested by oral administration in one experiment in mice and in one in hamsters. In mice, it produced liver-cell tumors in animals of both sexes. In hamsters of both sexes, it produced hepatomas, liver hemangiotheliomas and thyroid adenomas. In mice the effective intake of hexachlorobenzene that induced liver cell tumors was 12–24 mg/kg/bodyweight/day (Sax 1986).	
Mutagenicity	It was not mutagenic in yeast and did not induce dominant lethal effects in male rats (Sax 1986).	
Teratogenicity	Hexachlorobenzene is fetotoxic but produces no teratogenic effects (Sax 1986).	
Effects on plants	EC50, Brassica rapa sativa rapifera, > 1000 mg/kg, 14d EC50, Avena Sativa, > 1000 mg/kg, 14d (Anon. 1986b)	
EC50 values to algae, mg/l	0.03 < 0.03	3hr, Selenastrum capricornutum, photosynthesis 96hr, Selenastrim cappicornutum, growth (Calamari et al. 1983)
	0.01	96hr, grw, Scenedesmus subspicatus (Geyer et al. 1985)
	> 0.010	mg/kg, 4d,Scendesmus subspicatus (Anon. 1986b)
LC50 values to crustaceans, mg/l	< 0.03	24hr, Daphnia magna (Calamari et al. 1983)

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EC50 values to crustaceans, mg/l	0.016	14d, rpd, Daphnia magna (Calamari et al. 1983)
	0.5	14d, rpd, Daphnia magna (Hattori et al. 1984)
	0.025 0.0075	24hr, Daphnia magna 24hr, Daphnia magna (Anon. 1986b)
NOEC values to crustaceans, mg/l	0.005 0.0013	21d, rpd, Daphnia magna 21d, rdp, Daphnia magna (Anon. 1986b)
LC50 values to fishes, mg/l	< 0.03 < 0.03	48hr, Salmo gairdneri 48hr, Branchydanio rerio (Calamari et al. 1983)
	> 0.32	Poecilia (Verschueren 1983)
	50 22 14 12 12	96hr, Oncorhynchus kisutch, 7 °C 96hr, Pimephales promelas, 20 °C 96hr, Ictalurus punctatus, 20 °C 96hr, Lepomis macrochirus, 20 °C,hrd 96hr, Micropterus salmoides, 21 °C,hrd (Johnson & Finley 1980)
	> 5	48hr, Oryzias latipes (MITI 1992)
NOEC values to fishes, mg/l	> 0.005	mg/l, 14d, Brachydanio rerio (Anon. 1986b)
	0.00476	32d, Pimephales promelas (USEPA 1984)
Other information about water organisms	Tetrahymena pyriformis, growth, EC34, 10 d, 0.001 mg/l (Geike & Parasher 1976). Daphnia, EC0, 24hr, 0.025 mg/l (Dive et al. 1980). Micropterus, histological damage, 10 d, 0.003 mg/l (McCarty et al. 1985). No detectable effect: 0.050 mg/l, 48–72hr: Thalassiusira pseudonana; Dunaliella tertiolecta (Sax 1986).	
Other information	Human milk contains hexachlorobenzene, and infants may be exposed to relatively high concentrations from that source alone (Sax 1986).	

1127 • 1,4,5,6,7,7-Hexachlorobicyclo-(2,2,1)-5-heptene-2,3-dicarboxylic acid 115-28-6

Sumformula of the chemical	C9H4Cl6O4	
EINECS-number	2040789	
Water solubility, mg/l	0.0035	(MITI 1992)
Melting point, °C	208–210	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.22 < 2.1	6w, Cyprinus carpio, conc 0.01 mg/l 6w, Cyprinus carpio, conc 0.001 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	353	48hr, Oryzias latipes (MITI 1992)

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1128 • Hexachlorobutadiene

87-68-3

Sumformula of the chemical	C4Cl6	
Use	Solvent for natural rubber, synthetic rubber and other polymers; heat transfer liquid; transformer liquid; byproduct.	
State and appearance	Clear colourless liquid.	
Molecular weight	260.74	
Density, kg/m³	1675	
Vapour pressure, mmHg	22	100 °C
Water solubility, mg/l	4 5	20 °C 20 °C
Melting point, °C	-19– -22	
Boiling point, °C	210–220	
Log octanol/water coefficient, log Pow	4.78 4.8	(Anon. 1986b) (Anon. 1988)
Henry's law constant, Pa x m³/mol	110	(Anon. 1988)
Mobility	Equilibrium distribution: air water solid Theoretical distribution: > 99% in air (Nordic 1988).	*mass%* 78.02 2.06 19.93 (Anon. 1988).
Other information about degradation	Biodegradable (100% in 7 days) (Tabak et al. 1981).	
Other information about metabolism	When metabolized kidney damaging effects follow (Yang 1988).	
Bioconcentration factor, fishes	920-2300 29 > 10000 > 8000 6988	49d ,Carassius auratus 10d, Micropterus salmoides (Anon. 1986b) roach pike-perch (Goldbach et al. 1976) 32d, Pimephales promelas (USEPA 1984)
Bioconcentration factor, mollusca	> 18000	Sphaerium (Goldbach et al. 1976)
Bioconcentration factor, crustaceans	60	10d, Procambarus clarki (Anon. 1986b)
LD50 values to mammals in oral exposure, mg/kg	90 200–350 46–65	orl-rat, orl-gpg (Lewis & Sweet 1984) orl-rat 21d juv., orl-rat (Yang 1988)
LD50 values to mammals in non-oral exposure, mg/kg	1211 20	skn-rbt (Lewis & Sweet 1984) scu-rat, newborn (Yang 1988)
LCLo values to mammals in inhalation exposure, ppm	235	4hr, ihl-mus (Lewis & Sweet 1984)

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Other information about mammals	Rat: NOEL, orl, 30 d, 3 mg/kg/d; LOEL, orl, 30 d, 10 mg/kg/d; LOEL, orl, 2 years, 2 mg/kg/d (Kociba et al. 1977).
Carcinogenicity	Limited evidence of carcinogenicity in rats, tumours in kidneys (IARC 1979).
Mutagenicity	Metabolites seem to have mutagenic effects (Yang 1988).
Other information about birds	Coturnix japoniensis, NOEL, 90 d, 5 mg/kg/d (Schwetz et al. 1974).
LC50 values to crustaceans, mg/l	1.2 96hr, Nitocra (Bengtsson & Tarkpea 1983)
LC50 values to fishes, mg/l	0.09 96hr, Carassius auratus (Leeuwangh et al. 1975) 0.4 14 d, Poecilia reticulata (Könemann 1979) 0.326 Lepomis 0.102 Pimephales (USEPA 1980h) 0.16 14d, Poecilia (Hermens et al. 1985) 0.1 96hr, flow-through, Pimephales promelas 0.32 96hr, Salmo gairdneri (USEPA 1984)
EC50 values to fishes, mg/l	0.14 96hr, Salmo gairdneri (USEPA 1984)
LOEC values to fishes, mg/l	0.013 srv, grw, schr, Pimephales promelas (Benoit et al. 1982)
NOEC values to fishes, mg/l	0.0065 srv, grw, schr, Pimephales promelas (Benoit et al. 1982) 0.0065–0.013 32d, Pimephales promelas (USEPA 1984)
Other information	Estimated release: approximately 90% of production (Stephenson 1977).

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1129 • Hexachlorocyclohexane 608-73-1

Synonyms	BHC HCH
Molecular weight	290.82
Water solubility, mg/l	8 (MITI 1992)
Melting point, °C	112.5 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, mammals	37000 sea water/dolphin (Virtanen & Nuuja 1987)
Bioconcentration factor, fishes	327–893 (7.0) 10w, Cyprinus carpio, conc 0.0005 mg/l 49–223 (1.7) 8w, Cyprinus carpio, conc 0.0005 mg/l 395–777 (7.0) 10w, Cyprinus carpio, conc 0.00005 mg/l 48–336 (1.7) 8w, Cyprinus carpio, conc 0.00005 mg/l (MITI 1992)
Bioconcentration factor, crustaceans	142 sea water/zoopl. (Virtanen & Nuuja 1987)
LD50 values to mammals in oral exposure, mg/kg	100 orl-rat (Lewis & Sweet 1984)

LD50 values to mammals in non-oral exposure, mg/kg	900	skn-rat (Lewis & Sweet 1984)
	90	ukn-rat
	6000	β-HCH, ukn-rat (Virtanen & Nuuja 1987)
Health effects	Lethal dose to human: 7–15 g (Virtanen & Nuuja 1987).	
Carcinogenicity	Alfa-HCH: possible carcinogen (Virtanen & Nuuja 1987).	
LD50 values to birds in oral exposure, mg/kg	56	orl-brd
	75	orl-bwd (Lewis & Sweet 1984)
LC50 values to crustaceans, mg/l	2.45	96hr, Saccobranchus fossilis (Verma et al. 1982)
	0.0211	1d, Macrobrachium lamarrei
	0.0093	2d, Macrobrachium lamarrei
	0.0061	3d, Macrobrachium lamarrei (Mary et al. 1986)
LC50 values to fishes, mg/l	0.128	96hr, Cyprinus carpio (Singh et al. 1981)
	0.18	48hr, Oryzias latipes (MITI 1992)
Effects on the physiology of water organisms	Clarias batrachus, 2.0 mg/l, 28 d, change in hormone concentration (Singh & Singh 1987b).	

1130 • α-Hexachlorocyclohexane 319-84-6

Synonyms	α-HCH	
Use	Insecticide.	
Molecular weight	291	
Log octanol/water coefficient, log Pow	3.8	(Anon. 1988)
	3.8	(Anon. 1986b)
	3.72	(Schwarzenbach et al. 1983)
Henry's law constant, Pa x m^3/mol	0.016	(Anon. 1988)
Mobility	Equilibrium distribution:	
		mass %
	air	0.28
	water	50.67
	solid	49.05 (Anon. 1988).
Bioconcentration factor, fishes	140–1000	(Anon. 1986b)
Bioconcentration factor, crustaceans	60–475	Daphnia magna (Anon. 1986b)
Bioconcentration factor, algae	200	Chlorella pyrenoidosa (Anon. 1986b)
Carcinogenicity	Alfa-HCH: possible carcinogen (Virtanen & Nuuja 1987).	
LC50 values to crustaceans, mg/l	0.5	96hr, Artemia salina (Canton et al. 1978)
EC50 values to fishes, mg/l	1.31	96hr, Poecilia reticulata (Canton et al. 1978)
Other information about water organisms	Anabaena sp. 1.0–5.0 mg/l, 15–25 d, change in cell number of algae species including pre-exponential lag rate effects (Mathur & Saxena 1986).	

1131 • β-Hexachlorocyclohexane 319-85-7

Synonyms	β-HCH
Use	Insecticide.
Molecular weight	291
Log octanol/water coefficient, log Pow	3.8 (Anon. 1988) 3.78 (Anon. 1986b)
Henry's law constant, Pa x m³/mol	0.00023 (Anon. 1988)
Mobility	Equilibrium distribution *mass%* air 0.00 water 50.81 solid 49.19 (Anon. 1988).
Other information about water organisms	Anabaena sp., 0.1–2.5 mg/l, 15–30 d, change in cell number of algae species including pre-exponential lag rate effects (Mathur & Saxena 1986).

1132 • δ-Hexachlorocyclohexane 319-86-8

Other information about water organisms	Anabaena sp., 1.0 mg/l, 15 d, change in cell number of algae species including pre-exponential lag rate effects (Mathur & Saxena 1986).

1133 • Hexachlorocyclopentadiene 77-47-4

Synonyms	Perchlorocyclopentadiene
Sumformula of the chemical	C5Cl6
Use	Intermediate in manufacturing resins, dyes, pesticides, fungicides, pharmaceuticals and freons.
State and appearance	Colourless liquid.
Molecular weight	272.75
Specific gravity (water=1)	1.71
Vapour density (air=1)	9.42
Density, kg/m³	1710
Water solubility, mg/l	0.8–2.1, 25 °C
Melting point, °C	9.6
Boiling point, °C	234 239
Log octanol/water coefficient, log Pow	3.99 5.51 (Mackay 1982)
Other physicochemical properties	Nonflammable. Toxic compustion product: emits toxic and irritating fumes of phosgene, as well as carbon monoxide.
Photochemical degradation in water	Quick photolysis in water solution (half-life 4 minutes), forming water soluble ketones; e.g. pentachlorocyclopentenone and hexachlorocyclopentenone. Certain high molecular substances are also formed (Chou et al. 1987). Photomineralization, 17hr, 46% CO2 (Freitag et al. 1982).

Other information about degradation	Degradation products of special interest; hexachloroindenone (Chou et al. 1987).
Metabolism in mammals	Absorbed slightly through skin and through lungs. Absorbed badly in alimentary canal. Is preserved in liver, kidneys, ovaries and lungs (Fawell & Hunt 1988).
Bioconcentration factor, fishes	< 11 30d, Pimephales (Verschueren 1983) 1230 3d, Leuciscus (Freitag et al. 1982)
Other information about bioaccumulation	Active sludge, accumulation factor = 2350, 5 d (Freitag et al. 1982). Food chain contamination potential: Moderate. A model ecosystem study showed that HCCPD has considerable ecological stability and moderate biomagnification potential in aquatic organisms (Sax 1986).
LD50 values to mammals in oral exposure, mg/kg	113 orl-rat 500 orl-rat (Sax 1986)
LDLo values to mammals in oral exposure, mg/kg	420 orl-rbt (Sax 1986)
LDLo values to mammals in non-oral exposure, mg/kg	430 skn-rbt (Sax 1986)
LCLo values to mammals in inhalation exposure, ppm	1.5 ihl-mus, 7hr (Sax 1986)
TDLo values to mammals in oral exposure, mg/kg	975 orl-rbt, 6-18d preg, teratogenic effect (Sax 1986)
Other information about mammals	Mouse, ihl, 7 h – 216 d, lethal effect, 0.15 ppm (Sax 1986). Toxic effect in mouse and rat after 19 mg/kg/d for 13 weeks (Abdo et al. 1984).
Health effects	Strong irritation of eyes, nose and throat. Skin contact causes dermatitis, corrosion (Fawell & Hunt 1988). Degenerative changes in the brain, heart, adrenals, liver, kidney, and lungs are observed in severely poisoned animals by all routes of administration (Sax 1986). Direct contact: Contact with the skin can cause dermatitis, corrosion to tissues and can also be absorbed (Sax 1986). General sensation: Inhalation of vapours causes effects similar to inhalation of carbon tetrachloride, which include: irritation of eyes, nose, throat; headache, dizziness; nausea, vomiting, hematemesis; absominal cramps, diarrhea; nervousness; dyspnea; cyanosis; oliguria, proteinuria, hematuria; jaundice, hepatomegaly; optic neuritis; unconsciousness; coma; ventricular fibrillation (Sax 1986). Acute hazard level: This material is very toxic to humans (Sax 1986). Vapours cause similar toxic effects as carbon tetrachloride. Vapours can be absorbed through the intact skin. There is a narcotic action, and high enough concentrations can cause respiratory failure (Sax 1986). Skin and eye irritation data: skn, mky, 10 mg, severe; skn, rbt, 500 mg, 4hr, severe; eye, rbt, 20 mg, 24hr, severe; eye, rbt, 100 mg, 5 min, severe; skn, gpg, 20 mg, mild (Sax 1986).
Carcinogenicity	No information about carcinogenicity (Fawell & Hunt 1988).
Mutagenicity	Negative in Ames test and four other tests (Fawell & Hunt 1988).
Teratogenicity	No teratogenic or embryotoxic effects have been demonstrated (Fawell & Hunt 1988).
Effects on wastewater treatment	Not amenable to biological treatment at sewage treatment plant (Sax 1986).
LC50 values to crustaceans, mg/l	1 Daphnia (USEPA 1980i)

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LC50 values to fishes, mg/l	0.007	96hr, Pimephales promelas
	0.007	30d, larvae, juv, Pimephales promelas (Spehar et al. 1979)
	0.13	Lepomis
	0.105	Pimephales (USEPA 1980i)
	0.059	96hr, Pimephales (Sax 1986)

1134 • Hexachloroethane

67-72-1

Synonyms	Perchloroethane	
Use	Manufacturing smoke candles and grenades; by-product of industrial chlorination processes; plasticizer for cellulose esters.	
State and appearance	Solid rhombic crystals.	
Molecular weight	236.76	
Vapour pressure, mmHg	0.4	20 °C
Water solubility, mg/l	0.00005	22.3 °C (MITI 1992)
Boiling point, °C	186.8	(MITI 1992)
Henry's law constant, Pa x m³/mol	2267	calc. (Yaws et al. 1991)
Volatilization	Measured half-life for evaporation from 1 ppm aqueous solution at 25 °C: 40.7 min. (Verschueren 1983).	
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	756	32d, Pimephales promelas (USEPA 1984)
	1.4–8.5	6w, Cyprinus carpio, conc 0.005 mg/l
	1.0–6.8	6w, Cyprinus carpio, conc 0.0005 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	6000	orl-rat
	4970	orl-gpg (Lewis & Sweet 1984)
Carcinogenicity	NCI carcinogenesis bioassay completed: results positive, mus; results negative, rat (Lewis & Sweet 1984).	
EC50 values to microorganism, mg/l	8.3	Microtox (Tarkpea et al. 1986)
LC50 values to crustaceans, mg/l	8.1	48hr, Daphnia magna (LeBlanc 1980)
	2.9	48hr, unfed, Daphnia magna
	2.35	48hr, fed, Daphnia magna (USEPA 1984)
EC50 values to crustaceans, mg/l	2.1	48hr, unfed, Daphnia magna
	1.81	48hr, fed, Daphnia magna (USEPA 1984)

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LC50 values to fishes, mg/l	1.23 0.97 0.97 1.5 0.98 2.4 1.51 0.84 1.9	96hr, Pimephales promelas 96hr, Lepomis macrochirus 96hr, Salmo gairdneri (Phipps & Holcombe 1985) 96hr, Pimephales promelas (Veith et al. 1983) 96hr, Lepomis macrochirus (Buccafusco et al. 1981) 96hr, Cyprinodon variegatus (Heitmüller et al. 1981) 96hr, flow-through, Pimephales promelas 96hr, Salmo gairdneri (USEPA 1984) 48hr, Oryzias latipes (MITI 1992)
EC50 values to fishes, mg/l	0.84	96hr, Salmo gairdneri (USEPA 1984)
NOEC values to fishes, mg/l	0.069–0.207	32d, Pimephales promelas (USEPA 1984)

1135 • Hexachloronorbornadiene 3389-71-7

Use	Intermediate in the synthesis of isodrin and endrin.	
Log octanol/water coefficient, log Pow	5.28	(Mackay 1982)
LC50 values to fishes, mg/l	0.188 0.123 0.86 60.1	96hr, Pimephales promelas 30 d, Pimephales promelas 96hr, Pimephales promelas 96hr, Pimephales promelas (Spehar er al. 1979)

1136 • 1-Hexacosanol 506-52-5

Water solubility, mg/l	< 5	(MITI 1992)
Melting point, °C	82	(MITI 1992)
Boiling point, °C	305	20 mmHg (MITI 1992)
Total degradation in water	Biodegradation: 75% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	

1137 • n-Hexadecane 544-76-3

Bioconcentration factor, fishes	5.0–42.4 8.7–47.9	8w, Cyprinus carpio, conc 2.8 mg/l 8w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	1600	48hr, Oryzias latipes (MITI 1992)

1138 • 1-Hexadecene 629-73-2

Sumformula of the chemical	C16H32
Water solubility, mg/l	< 100 (MITI 1992)
Melting point, °C	3.9 (MITI 1992)
Boiling point, °C	286–287 (MITI 1992)
Total degradation in water	Biodegradation: 55–77% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

1139 • Hexadecylpyridiniumbromide 140-72-7

Synonyms	Cetylpyridiniumbromide
Use	Surface active agent; germicide.
State and appearance	Cream-coloured waxy solid.
Other information about degradation	Biodegradation: at 18 mg/l (inoculum = sewage) lag period = 6 days; after 17 days complete degradation (Verschueren 1983).
Effects on microorganisms	Staphylococcus aureus: at 20 mg/l bacteriolytic action after 5 hours; Escherichia coli: at 20 mg/l slight reduction of growth rate, at 5 mg/l no significant reduction of growth rate (Verschueren 1983).

1140 • Hexadecyltrimethylammoniumbromide 57-09-0

Synonyms	Cetyltrimethylammoniumbromide
Sumformula of the chemical	C19H42NBr
Use	Surface active agent; germicide.
State and appearance	White powder.
Molecular weight	364.46
Degradation point, °C	> 230 °C
Other information about degradation	Biodegradation: at 15 mg/l: not adapted sewage: lag time: 2 days, complete degradation after 4 days; adapted sewage: complete degradation after 2 days (Verschueren 1983).
Effects on microorganisms	Escherichia coli: at 20 mg/l no significant reduction of growth rate (Verschueren 1983).
Other information about water organisms	Poteriochromonas malhamensis; 4.38 mg/l, 3d, lethal (100% mortality or 0% survival including algicidal and herbicidal effects) (Roderer 1987).

1141 • Hexadecyltrimethylammoniumchloride 112-02-7

Synonyms	Cetyltrimethylammoniumchloride
Sumformula of the chemical	C19H42NCl
Use	Surface active agent.

Other information about degradation	Degradation; at 15 mg/l: not adapted sewage: lag time: 4 days, complete degradation after 7 days; adapted sewage: at 18 mg/l, complete degradation after 2 days (Verschueren 1983).
Effects on microorganisms	Staphylococcus aureus: at 20 mg/l no growth (Verschueren 1983).

1142 • 2,4-Hexadienic acid

110-44-1

Synonyms	2,4-Hexadienoic acid Sorbic acid	
Sumformula of the chemical	C6H8O2	
Water solubility, mg/l	950	(MITI 1992)
Melting point, °C	134.5	(MITI 1992)
pKa	4.6	est. Sangster 1989
Log octanol/water coefficient, log Pow	1.33	(Sangster 1989)
Total degradation in water	Biodegradation: 83% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	

1143 • 1,1,1,3,3,3-Hexafluoro-2-propanol

920-66-1

Water solubility, mg/l	> 20 000 (MITI 1992)	
Total degradation in water	Biodegradation: 0% by TOC and GC period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992)	
Bioconcentration factor, fishes	1.1–1.4 1.3–2.7	6w, Cyprinus carpio, conc 1 mg/l 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	270	48hr, Oryzias latipes (MITI 1992)

1144 • Hexahydro-1,3,5-tris-(2-hydroxyethyl)-1,3,5-triazine

4719-04-4

Sumformula of the chemical	C9H21N3O3
Water solubility, mg/l	> 3000 (MITI 1992)

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Total degradation in water	Biodegradation: 89–95% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

1145 • Hexamethyl phosphoric triamide 680-31-9

Sumformula of the chemical	C6H18OPN3
Water solubility, mg/l	> 100000 (MITI 1992)
Melting point, °C	7 (MITI 1992)
Log octanol/water coefficient, log Pow	0.13 (MITI 1992)
Total degradation in water	Biodegradation: 0–1% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l MITI 1992.
Bioconcentration factor, fishes	< 0.05 6w, Cyprinus carpio, conc 2 mg/l < 0.5 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 1000 48hr, Oryzias latipes (MITI 1992)

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1146 • Hexamethylbenzene 87-85-4

Sumformula of the chemical	C12H18
Log octanol/water coefficient, log Pow	4.75 (Sangster 1989)

1147 • Hexamethylenediamine 124-09-4

Synonyms	1,6-Hexanediamine
Melting point, °C	42 (MITI 1992)
Boiling point, °C	42 (MITI 1992)
Total degradation in water	Biodegradation: 56% by BOD (on the upward trend) period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
LD50 values to birds in oral exposure, mg/kg	> 101 orl-Agelaius phoeniceus (Schafer et al. 1983)

1148 • Hexamethylenetetramine

100-97-0

Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LC50 values to crustaceans, mg/l	92500	96hr, 10 °C, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	> 10000	96hr, 10 °C, Alburnus alburnus (Linden et al. 1979)

1149 • N-Hexamethylolmelamine

3089-11-0

Sumformula of the chemical	C15H30N6O6	
Total degradation in water	Biodegradation: 4.6% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.2 < 1.9	6w, Cyprinus carpio, conc 1 mg/l 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
LC50 values to fishes, mg/l	680	48hr, Oryzias latipes (MITI 1992)

1150 • n-Hexane

110-54-3

Water solubility, mg/l	21	
Boiling point, °C	69	
Log octanol/water coefficient, log Pow	4	(Sangster 1989)
Henry's law constant, Pa x m³/mol	130800	calc. (Yaws et al. 1991)
Volatilization	Relative volatility (nBuAc=1) = 7.2	
LCLo values to mammals in inhalation exposure, mg/kg	120000	mus
LC50 values to fishes, mg/l	4	24hr, Carassius auratus (Anon. 1975)

1151 • 1,2,6-Hexanetriol

106-69-4

LC50 values to crustaceans, mg/l	13700	96hr, 10 °C, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	> 10000	96hr, 10 °C, Alburnus alburnus (Linden et al. 1979)

1152 • 1-Hexanol

111-27-3

Synonyms	Hexanol n-Hexanol Hexyl alcohol Amyl carbinol
Sumformula of the chemical	C6H14O

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Use	Pharmaceuticals solvent, plasticizer, intermediate for textile and leather finishing agents.
State and appearance	Colourless liquid.
Odour	Quality: sweet, alcohol Hedonic tone: pleasant Threshold odour concentration absolute: 0.01 ppm 50% recognition: 0.09 ppm 100% recognition: 0.09 ppm Odour index 100% recognition: 14 666 (Hellman & Small 1974).
Specific gravity (water=1)	0.8186
Boiling point, °C	157.2
Flashing point, °C	65
Log octanol/water coefficient, log Pow	2 (Anon. 1986) 2.03 (Sangster 1989)
Henry's law constant, Pa x m³/mol	1.897 calc. (Yaws et al. 1991)
Other physicochemical properties	Sligthly soluble in water, soluble in alcohol and ether. Combustible. Autoign temperature 292 °C.
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 62 mg/l (Bringmann & Kühn 1980a).
EC50 values to microorganism, mg/l	68 15 min Microtox (Hermens et al. 1985) 2350 Biodegradation inhibition (Vaishnav 1986)
LC50 values to fishes, mg/l	120 96hr, 10 °C, Alburnus alburnus (Linden et al. 1979)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 30 mg/l protozoa (Entosiphon sulcatum): 75 mg/l (Bringmann & Kühn 1980a).

1153 • 2-Hexanol 626-93-7

Sumformula of the chemical	C6H14O
Log octanol/water coefficient, log Pow	1.76 (Sangster 1989)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 63 mg/l (Bringmann & Kühn 1980a).
LOEC values to algae, mg/l	72 rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a) 32 rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to fishes, mg/l	340 96hr, Branchydanio rerio 287–332 48hr, Leuciscus idus (Wellens 1982)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 72 mg/l protozoa (Entosiphon sulcatum): 116 mg/l (Bringmann & Kühn 1980a).

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1154 • 3-Hexanol

623-37-0

Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 105 mg/l (Bringmann & Kühn 1980a).
LOEC values to algae, mg/l	32 rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976) 63 rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 63 mg/l protozoa (Entosiphon sulcatum): 182 mg/l (Bringmann & Kühn 1980a).

1155 • 2-Hexanone

591-78-6

Synonyms	Methyl butyl ketone Butyl methyl ketone	
Sumformula of the chemical	C4H9COCH3	
Use	Solvent.	
State and appearance	Colourless liquid.	
Odour	Odour Threshold: 0.28–0.35 mg/m³ (Verschueren 1983).	
Molecular weight	100.2	
Specific gravity (water=1)	0.83	at 0/4 °C
Vapour density (air=1)	3.45	
Vapour pressure, mmHg	2	at 20 °C
Water solubility, mg/l	34400	20 °C
Melting point, °C	-57	
Boiling point, °C	128	
Log octanol/water coefficient, log Pow	1.38	(Sangster 1989)
Volatilization	Relative volatility (nBuAc=1) = 1.06	
LD50 values to mammals in oral exposure, mg/kg	2590	orl-rat
EC50 values to microorganism, mg/l	5509	Biodegradation inhibition (Vaishnav 1986)

1156 • 1-Hexene

592-41-6

Sumformula of the chemical	C6H12	
Water solubility, mg/l	54	(MITI 1992)
Melting point, °C	-140– -139	(MITI 1992)
Boiling point, °C	63.35	(MITI 1992)
Total degradation in water	Biodegradation: 67–98% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

1157 • Hexyl acetate 123-92-2

Use	Solvent.	
Water solubility, mg/l	1600	20 °C
Boiling point, °C	142	
LD50 values to mammals in oral exposure, mg/kg	6160	orl-rat

1158 • 4'-n-Hexyl-4-cyanobiphenyl 41122-70-7

Sumformula of the chemical	C19H21N	
Water solubility, mg/l	1.5	(MITI 1992)
Log octanol/water coefficient, log Pow	5.35	(MITI 1992)
Total degradation in water	Biodegradation: 0–5% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	1570–6160 1710–4920	8w, Cyprinus carpio, conc 0.05 mg/l 8w, Cyprinus carpio, conc 0.005 mg/l (MITI 1992)
LC50 values to fishes, mg/l	1.16	48hr, Oryzias latipes (MITI 1992)

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1159 • n-Hexylbenzene 1077-16-3

Sumformula of the chemical	C12H18	
Log octanol/water coefficient, log Pow	5.52	(Sangster 1989)

1160 • Hexyleneglycol 107-41-5

Synonyms	2-Methyl-2,4-pentanediol 2,4-Dihydroxy-2-methylpentane 1,2-Hexanediol Hexylene glycol Isol 2-Methylpentane-2,4-diol α,α,α-Trimethyltrimethyleneglycol	
Sumformula of the chemical	C6H14O2	
Use	Solvent.	
Boiling point, °C	198.3	(MITI 1992)
Volatilization	Relative volatility (nBuAc=1) = 0.003	
Chemical oxygen demand, g O2/g	2.2	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g O2/g	0.02	5 days (Bridie et al. 1979)

Total degradation in water	Biodegradation: 35–76% by BOD period:28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	2800 3097 3700 3200	orl-gpg orl-mus orl-rat orl-rbt (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	1299 13 8560	ipr-mus scu-rbt skn-rbt (Sweet 1987)
LDLo values to mammals in non-oral exposure, mg/kg	1500	ipr-rat (Sweet 1987)
TCLo values to mammals in inhalation exposure, ppm	50	ihl-hmn, 15 min. (Sweet 1987)
LC50 values to crustaceans, mg/l	7600	96hr, 10 °C, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	10000 > 5000 8000	96hr, Menidia audens (Verschueren 1983) 24hr, Carassius auratus (Bridie et al. 1979) 96hr, 10 °C, Alburnus alburnus (Linden et al. 1979)

1161 • 4-(Hexyloxy)phenol

18979-55-0

Other information about water organisms	Tetrahymena pyriformis, EC50, grw, 2 d, 4.37 mg/l (Schultz 1987).

1162 • p-Hexylphenol

2446-69-7

LC50 values to fishes, mg/l	0.19	96hr, Salmo salar (McLeese et al. 1981)

1163 • Hydrazine

302-01-2

Use	In industry (strong reducing and antioxidant property).	
State and appearance	Liquid.	
Molecular weight	32.06	
Vapour pressure, mmHg	16	20 °C
Melting point, °C	2	
Boiling point, °C	113	
LD50 values to mammals in oral exposure, mg/kg	60	orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	91	skn-rbt (Lewis & Sweet 1984)

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LC50 values to mammals in inhalation exposure, mg/m³	758	4hr, ihl-rat (Lewis & Sweet 1984)
LC50 values to mammals in inhalation exposure, ppm	570 252	4hr, ihl-rat (Lewis & Sweet 1984) 4hr, ihl-mus (Lewis & Sweet 1984)
TCLo values to mammals in inhalation exposure, ppm	1	6hr, ihl-rat (Lewis & Sweet 1984)
Effects on plants	Seeds of two rice types were treated for 6 hours with 1.5% hydrazine in tris-maleate buffer at 5 different pH-levels —reduction in shoot length, chlorophyll mutations (Augustine et al. 1975).	
EC50 values to crustaceans, mg/l	0.16 0.19	srv, 48hr, Daphnia pulex srv, 48hr, Daphnia pulex (Velte 1984)
LC50 values to fishes, mg/l	0.61 3.85 1.17 1.0-1.6	sfd,96hr, Poecilia reticulata hrd,96hr, Poecilia reticulata (Slonium 1977) 96hr, Lepomis macrochirus 96hr, Lepomis macrochirus (Hunt et al. 1981)
EC50 values to fishes, mg/l	6	96hr, Pimephales promelas (Velte 1984)

1164 • Hydrofluoric acid 7664-39-3

Synonyms	Hydrogen fluoride Anhydrous hydrofluoric acid Anhydrous hydrogen fluoride Fluoric acid Hydrofluoride	
Sumformula of the chemical	HF	
Purity, %	30–80% HF aqueous 99% anhydrous	
Use	Metal trades; glass; polish; chemical industry. HF is used in metal industry; in manufacturing of fluorine containing plastic and polymers (teflon) and freons.	
State and appearance	Colourless.	
Molecular weight	20.01	
Specific gravity (water=1)	0.991	
Vapour density (air=1)	0.71	
Vapour pressure, mmHg	358	0 °C
Melting point, °C	-83.1 -92.3	
Boiling point, °C	112.2 19.5	azeotrope with water
pKa	3.17	
Other bindings	Soil can bind fluorides tightly if pH is > 6.5; high calcium content will also immobilize fluorides (Sax 1986).	
Other physicochemical properties	Solubility: miscible.	
Other information about degradation	Natural alkalinity slowly dissipates acidity (Sax 1986).	

LC50 values to mammals in inhalation exposure, ppm	1310 1278 500 1780 4342 342	ihl-rat 1hr, ihl-rat 1hr, ihl-mus 1hr, ihl-mky 15min, ihl-gpg (Sax 1986) 1hr, ihl-mus (Sweet 1987)
LDLo values to mammals in oral exposure, mg/kg	80	orl-gpg (Sax 1986)
LDLo values to mammals in non-oral exposure, mg/kg	100 25	scu-gpg ipr-rat (Sax 1986)
LCLo values to mammals in inhalation exposure, mg/kg	1000 260	ihl-gpg ihl-gpg (Sax 1986)
LCLo values to mammals in inhalation exposure, ppm	50 342 1774 4327	30 min, ihl-hmn 1hr, ihl-mus 1hr, ihl-mky 15min, ihl-gpg (Sax 1986) 30 min, ihl-hmn 1hr, ihl-mus 1hr, ihl-mky 15min, ihl-gpg (Sax 1986) 30 min, ihl-hmn 1hr, ihl-mus 1hr, ihl-mky 15min, ihl-gpg (Sax 1986) 30 min, ihl-hmn 1hr, ihl-mus 1hr, ihl-mky 15min, ihl-gpg (Sax 1986)
TCLo values to mammals in inhalation exposure, mg/kg	0.47 4.98 100	4hr, ihl-rat, 1-22d preg. 4hr, ihl-rat, 1-22d preg. teratogenic effect (Sax 1986) 1min, ihl-man, sense organs and special senses lungs, thorax or respiration (Sweet 1987)
TCLo values to mammals in inhalation exposure, ppm	110	1 min, ihl-man (Sax 1986)
Health effects	Direct contact: highly irritable; severe and painful injury on contact. Skin, eyes; gangrene of affected areas may follow. General sensation: Severe irritation to eyes resulting in visual defects. Skin contact results in pungent irritating odour. Severe burns. Recognition odour 0.03 mg/m³. Dose effect relations: 3 ppm = good warning properties; MAC 8hr, 10 ppm, MAC 0.5–1hr, 30 ppm sour taste smarting eyes; 60 ppm, burn pain may be delayed up to 1hr; apparent irritation of nose and eyes; 120 ppm irritation of skin, respiratory system; vapours can cause ulcers of respiratory tract; 50–250 ppm dangerous with short exposure; 1500 ppm fatal to animals in tract. 5 min concentration of 50–250 ppm can be dangerous even for brief exposures (Sax 1986).	

Mutagenicity	dnd, dmg, ihl, 1300 ppb, 6 w; sln, dmg, ihl, 2900 ppb (Sax 1986). cyt, rat, ihl, 1 mg/m³, 6hr (Sweet 1987). Exposure to hydrogen fluoride induces increased frequence of lethal and sterile mutations both in plants and in banana flies (Borg 1976).
Effects on amphibia	LDLo, 112 mg/kg, scu, frog (Sax 1986).
Effects on plants	Fluorides can be damaging to plants when present in acid soils (Sax 1986).
LC50 values to crustaceans, mg/l	> 300 NaF, 48hr, shrimp (Sax 1986)
Other information about water organisms	60 mg/l, fish, lethal; 40 mg/l, fish, harmful (Sax 1986). 0.9–4.5 mg/l NaF, lobster, not toxic; 100 mg/l NaF, mullet, ambasis, safgha, terapon, prawn, jaruba, no effect, 96hr; 7.2 mg/l NaF, 108hr, brown mussels, toxic effect; 52 mg/l NaF, 72 d, mullet, crab, physical deterioration; 52 mg/l NaF, 72 d, shrimp, affects reproduction (Sax 1986).
Other information	Strong irritant. Highly toxic via ingestion or inhalation. Moderately toxic with chronic exposure. Emits toxic vapours when heated to decomposition (Sax 1986). Air pollution high (Sax 1986).

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1165 • Hydrogen cyanide 74-90-8

Synonyms	HCN	
State and appearance	Colourless gas or liquid.	
Molecular weight	27.03	
Vapour pressure, mmHg	620	20 °C
Melting point, °C	-13.3	
Boiling point, °C	25.6	
LD50 values to mammals in oral exposure, mg/kg	3.7	orl-mus (Lewis & Sweet 1984)
LDLo values to mammals in oral exposure, mg/kg	0.57 2	orl-hmn orl-pig (Lewis & Sweet 1984)
LCLo values to mammals in inhalation exposure, mg/kg	120	1hr, ihl-hmn (Lewis & Sweet 1984)
LCLo values to mammals in inhalation exposure, ppm	323	5 min, ihl-mus (Lewis & Sweet 1984)
LC50 values to crustaceans, mg/l	0.17	96hr, Gammarus pseudolimnaeous (Verschueren 1983)
LC50 values to fishes, mg/l	0.125 0.057	96hr, Pimephales promelas 96hr, Salmo gairdneri (Broderius & Smith 1979)

1166 • Hydrogen peroxide * 90% 7722-84-1

Synonyms	Dihydrogen dioxide Hydrogen dioxide Hydroperoxide Peroxide	
Sumformula of the chemical	H2O2	
Molecular weight	34.02	
LD50 values to mammals in oral exposure, mg/kg	2000	orl-mus (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	25 15000 4060	ivn-mus ivn-rbt skn-rat (Sweet 1987)
LC50 values to mammals in inhalation exposure, mg/m³	2000	multiple-rat (Sweet 1987)
LDLo values to mammals in non-oral exposure, mg/kg	2000 500	skn-pig skn-rbt (Sweet 1987)
LCLo values to mammals in inhalation exposure, ppm	227	ihl-mus (Sweet 1987)
TDLo values to mammals in oral exposure, mg/kg	144000	orl-mus, tumorigenic (Sweet 1987)
Mutagenicity	Cytogenic analysis: ham, ovr, 1 mmol/l; ham, lug, 0.1 mmol/l; ham, emb, 0.1 mmol/l; ham, fbr, 250 mg/l; mus, Ascites tumor; 10 mmol/l; mus, emb, 0.01 mmol/l; DNA damage; bcs, 50 mmol/l; ham, lug, 0.353 mmol/l; hmn, fbr, 0.028 mmol/l; hmn, cell types, 0.1 mmol/l; hmn, lym, 0.1 mmol/l; mam, lym, 0.6 mmol/l; mus, cell types, 0.1 mmol/l; mus, cell types. 0.001 mmol/l DNA inhibition: hmn, cell types, 1.2 mmol/l; hmn, fbr, 1 mg/l; mus, cell types, 0.04 mmol/l; DNA repair: esc, 10 µl, well, 16hr; unscheduled DNA synthesis; hmn, fbr, 1 mmol/l; hmn, lug, 0.6 mg/l; gene conversion and mitotic recombination: smc, 5 pph;	

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	microbial mutation without S9: bcsm 5 ppm; esc, 5 pph; nsc, 210 mmol/l, 30 min; microorganisms, 6 ppm; smc, 10 mg/l; ssp, 2820 mmol/l; microsomal assay: sat, 6 µg/plate; sister chromatid exchange: ham, lug, 40 µmol/l (Sweet 1987).

1167 • Hydrogen sulfide 7783-06-4

Sumformula of the chemical	H_2S	
State and appearance	Colourless gas.	
Molecular weight	34.08	
Melting point, °C	-83.8– -85.5	
Boiling point, °C	-60.2	
LC50 values to mammals in inhalation exposure, mg/m³	1	8hr, ihl-gpg (Lewis & Sweet 1984)
LC50 values to mammals in inhalation exposure, ppm	444 600 673 800	0.63 mg/l, ihl-rat (Lewis & Sweet 1984) 30min., ihl-hmn (Lewis & Sweet 1984) 1hr, ihl-mus (Lewis & Sweet 1984) 5 min., ihl-mam (Lewis & Sweet 1984)
LCLo values to mammals in inhalation exposure, mg/kg	1	8hr, ihl-gpg (Lewis & Sweet 1984)
LCLo values to mammals in inhalation exposure, ppm	600	30 min, ihl-hmn (Lewis & Sweet 1984) 30 min, ihl-hmn (Lewis & Sweet 1984)
Effects on plants	Continuous fumigation of Douglas fir (Pseudotsuga menziesii) seedlings with 100 ppb (0.139 mg/m³) H_2S caused slight 'tip burn' of needles, but 300 ppb (0.417 mg/m³) caused very extensive foliar injury (Thompson & Kats 1978).	
LC50 values to crustaceans, mg/l	0.11	96hr, Asellus (Oseid et al. 1974)
LC50 values to fishes, mg/l	0.007–0.55 0.019 0.013 0.022–0.031 0.026 0.037	6–24 °C, 96hr, Pimephales promelas (Smith & Oseid 1975) 72hr, eggs, Lepomis macrochirus 96hr, Lepomis macrochirus (Smith Jr. et al. 1976) 96hr, Salvelinus fontinalis (Smith & Oseid 1975) 96hr, Esox lucius 96hr, eggs, Esox lucius (Adelman & Smith Jr. 1972)
Other information	The toxicity of hydrogen sulfide increases when the temperature decreases (Smith & Oseid 1975).	

1168 • Hydroquinone 123-31-9

Synonyms	1,4-Dihydroxybenzene p-Hydroxyphenol 1,4-Benzenediol

Use	Photographic developer and oxidation inhibitor; dye intermediate; medicine; inhibitor of polymerization.
State and appearance	Hexagonal prisms.
Molecular weight	110.12
Vapour pressure, mmHg	4 150 °C
Water solubility, mg/l	70000 25 °C 5.8% (MITI 1992)
Melting point, °C	172
Boiling point, °C	218.2
Total degradation in water	Biodegradation: 70% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	320 orl-rat 70 orl-cat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	5970 skn-mam (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	300 orl-pgn (Lewis & Sweet 1984)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 58 mg/l (Bringmann & Kühn 1980a)
LOEC values to algae, mg/l	0.93 Scenedesmus quadricauda, Bringmann & (Kühn 1980a)
LC50 values to crustaceans, mg/l	0.05 48hr, Daphnia magna (Könemann 1979)
LC50 values to fishes, mg/l	0.097 96hr, Salmo gairdneri 0.044 96hr, Pimephales promelas (DeGraeve et al. 1980) 0.17 96hr, Branchydanio rerio 0.16 48hr, Leuciscus idus (Wellens 1982)
Other information about water organisms	Daphnia pulex: 0.001 mol/l, srv, 0.07 days (Stom et al. 1986). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 0.93 mg/l protozoa (Entosiphon sulcatum): 11 mg/l (Bringmann & Kühn 1980a)

1169 • Hydroquinonemonobenzylether 103-16-2

LC50 values to fishes, mg/l	2.5 48hr, Carassius auratus (McKee & Wolf 1963)

GHI

1170 • 7-Hydroxy-1,3-naphthalene disulfonic acid dipotassium salt

842-18-2

Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.1 < 1.0	6w, Cyprinus carpio, conc 1 mg/l 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 1000	48hr, Oryzias latipes (MITI 1992)

1171 •2-Hydroxy-1,7,7-trimethyl bicyclo(2,2,1)heptane

507-70-7

Water solubility, mg/l	480	(MITI 1992)
Melting point, °C	197–200	(MITI 1992)
Log octanol/water coefficient, log Pow	2.69	(MITI 1992)
Total degradation in water	Biodegradation: 95–99% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

1172 • 3-Hydroxy-2-naphthoic acid

92-70-6

Total degradation in water	Biodegradation: 1.3% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.5 < 4	6w, Cyprinus carpio, conc 1 mg/l 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LD50 values to birds in oral exposure, mg/kg	> 68.0	orl-Agelaius phoeniceus (Schafer et al. 1983)
LC50 values to fishes, mg/l	127	48hr, Oryzias latipes (MITI 1992)

GHI

1173 • 2-(2'-Hydroxy-3',5'-di-t-butylphenyl)-5-chlorobenzotriazole 3864-99-1

Melting point, °C	154–158 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.4–12.2 6w, Cyprinus carpio, conc 0.4 mg/l < 4–15.9 6w, Cyprinus carpio, conc 0.04 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	94 48hr, Oryzias latipes (MITI 1992)

1174 • 2-Hydroxy-4-methoxybenzophenone 131-57-7

Synonyms	Methanone (2-hydroxy-4-methoxyphenyl)phenyl-
Sumformula of the chemical	C14H12O3
EINECS-number	2050315
Water solubility, mg/l	< 100 (MITI 1992)
Melting point, °C	63–65 (MITI 1992)
Log octanol/water coefficient, log Pow	3.79 (MITI 1992)
Total degradation in water	Biodegradation: 3–4% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	39–160 10w, Cyprinus carpio, conc 0.1 mg/l 33–156 10w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
LC50 values to fishes, mg/l	8.48 48hr, Oryzias latipes (MITI 1992)

1175 • 4-(4-Hydroxy-4-methyl-pentyl)-3-cyclohexenecarbaldehyde 31906-04-4

Sumformula of the chemical	C13H22O2
Water solubility, mg/l	6100 (MITI 1992)
Melting point, °C	< -30 (MITI 1992)
Total degradation in water	Biodegradation: 52–66% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

GHI

1176 • 3-Hydroxy-5-hydroxymethyl-2-methyl isonicotinaldehyde — 66-72-8

Sumformula of the chemical	C8H9NO3
EINECS-number	2006308
Water solubility, mg/l	> 10000 (MITI 1992)
Melting point, °C	178 (MITI 1992)
Total degradation in water	Biodegradation: 77% by BOD (NO2) period: 21d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

1177 • 1-Hydroxyanthraquinone — 129-43-1

Sumformula of the chemical	C14H8O3
Water solubility, mg/l	2.4 (MITI 1992)
Melting point, °C	196–198 (MITI 1992)
Log octanol/water coefficient, log Pow	3.53 Anon. 1986 4.04 (MITI 1992)
Total degradation in water	Biodegradation: 1–5% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	55–318 8w, Cyprinus carpio, conc 0.05 mg/l 62–297 8w, Cyprinus carpio, conc 0.005 mg/l (MITI 1992)
LC50 values to fishes, mg/l	6.78 48hr, Oryzias latipes (MITI 1992)

1178 • 3-Hydroxybenzenemethanol — 620-24-6

Other information about water organisms	Tetrahymena pyriformis, 1371 mg/l, EC50, grw, 2 d (Schultz 1987).

1179 • 3-Hydroxybenzonitrile — 873-62-1

Other information about water organisms	Tetrahymena pyriformis, 138.22 mg/l, EC50, grw, 2 d (Schultz 1987).

1180 • 2-Hydroxyethyl acrylate — 818-61-1

Sumformula of the chemical	C5H8O3
Water solubility, mg/l	> 100000(MITI 1992)

GHI

Melting point, °C	< -10 (MITI 1992)
Boiling point, °C	201.8–204.4 (760 mmHg) (MITI 1992)
Total degradation in water	Biodegradation: 76–80% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

1181 • 2-Hydroxyethyl methacrylate 868-77-9

Sumformula of the chemical	C6H10
Water solubility, mg/l	> 100000 (MITI 1992)
Melting point, °C	< -10 (MITI 1992)
Boiling point, °C	211 (MITI 1992)
Total degradation in water	Biodegradation: 92–100% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

1182 • 9-Hydroxyfluorene 1689-64-1

EC50 values to algae, mg/l	27	rpd, 72hr, Dunaliella bioculata (Heldal et al. 1984)

1183 • N-(Hydroxymethyl)alkane-(C=14-18)amide

3370-35-2 *C17

24537-30-2 *C15

101453-46-7 *C13

Water solubility, mg/l	< 10 (MITI 1992)
Melting point, °C	111 (MITI 1992)
Total degradation in water	Biodegradation: 83–89% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

1184 • 2-((Hydroxymethyl)amino) ethanol 34375-28-5

Water solubility, mg/l	> 1 (MITI 1992)
Total degradation in water	Biodegradation: 68% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

1185 • N-(2-Hydroxyphenyl)acetoamide 614-80-2

Sumformula of the chemical	C8H9O2N
Water solubility, mg/l	880 (MITI 1992)
Melting point, °C	207–209 (MITI 1992)
Total degradation in water	Biodegradation: 69–89% (NH3) by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).

1186 • 2-Hydroxypyridine 142-08-5

Synonyms	2(1H)-Pyridone 2-Oxopyridine 2-Pyridinol 2-Pyridinone 2(1H)-Pyridinone α-Pyridone 2-Pyridone
Sumformula of the chemical	C5H5NO
Water solubility, mg/l	> 3000 (MITI 1992)
Melting point, °C	106–107 (MITI 1992)
Boiling point, °C	280–281 (MITI 1992)
Total degradation in water	Biodegradation: 51–58% (NO2) by BOD 62–74% (NH3) by BOD period: 21d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
LD50 values to mammals in non-oral exposure, mg/kg	410 ipr-mus 750 ivn-mus (Sweet 1987)
LD50 values to birds in oral exposure, mg/kg	> 1000 orl-Agelaius phoeniceus > 1000 orl-Sturnus vulgaris > 1000 orl-Coturnix coturnix 1000 orl-Passer domesticus (Schafer et al. 1983)
Other information about water organisms	Tetrahymena pyriformis, EC50, grw, 2.5 d, 3877.2 mg/l (Schultz et al. 1987).

1187 • 3-Hydroxypyridine 109-00-2

Synonyms	3-Pyridinol β-Hydroxypyridine 3-Pyridol
Sumformula of the chemical	C5H5NO

GHI

Water solubility, mg/l	> 3000 (MITI 1992)
Melting point, °C	129 (MITI 1992)
Total degradation in water	Biodegradation: 72% (NO2) by BOD 93% (NH3) by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
LD50 values to mammals in non-oral exposure, mg/kg	1822 ipr-mus (Sweet 1987)
LD50 values to birds in oral exposure, mg/kg	750 orl-wild bird (Sweet 1987) 750 orl-Agelaius phoeniceus > 1000 orl-Sturnus vulgaris > 1000 orl-Coturnix coturnix 1000 orl-Passer domesticus (Schafer et al. 1983)
Other information about water organisms	Tetrahymena pyriformis, EC50, grw, 2.5 d, 432.7 mg/l (Schultz et al. 1987).

1188 • 4-Hydroxypyridine

626-64-2

Water solubility, mg/l	> 3000 (MITI 1992)
Melting point, °C	148.5 (MITI 1992)
Boiling point, °C	257–260 10 mmHg (MITI 1992)
Total degradation in water	Biodegradation: 44–66% (NO2) by BOD 53–81% (NH4) by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

1189 • 12-Hydroxystearic acid

106-14-9

Sumformula of the chemical	C18H3603
EINECS-number	2033661
Water solubility, mg/l	< 100 (MITI 1992)
Melting point, °C	78.1 (MITI 1992)
Total degradation in water	Biodegradation: 91–98% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

GHI

1190 • Hymexazol

10004-44-1

Use	Active ingredient in fungicides.	
LC50 values to fishes	> 40	48hr, Cyprinus carpio (Pesticide Manual 1983)

1191 • Imidan

732-11-6

Synonyms	0,0-Dimethyl-S-phthalimidemethyl-phosphorodithioate Phosmet	
Use	Acaricide, insecticide.	
Molecular weight	317.33	
Water solubility, mg/l	25	25 °C
LD50 values to mammals in oral exposure, mg/kg	147 26	orl-rat orl-mus (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	1550	skn-rat (Lewis & Sweet 1984)
LC50 values to mammals in inhalation exposure, mg/m³	54	4hr, ihl-rat (Lewis & Sweet 1984)
TCLo values to mammals in inhalation exposure, mg/kg	2	ihl-hmn (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	18 17.8 > 100	orl-bwd (Lewis & Sweet 1984) orl-Agelaius phoeniceus orl-Sturnus vulgaris (Schafer et al. 1983)
LC50 values to crustaceans, mg/l	0.025 0.0024 2.75 0.84	Daphnia pulex (Nishiuchi & Hashimoto 1967) 48hr, Gammarus pseudolimnaeus (Julin & Sanders 1977) 24hr, Daphnia magna 48hr, Daphnia magna (Ardo 1974)
LC50 values to fishes, mg/l	0.56 0.07 0.15 11 5.3	96hr, Salmo gairderi 96hr, Lepomis macrochirus 96hr, Oncorhynchys tschawytscha 96hr, Ictalurus punctatus (Julin & Sanders 1977) 48hr, Cyprinus carpio (Nishiuchi & Hashimoto 1967)

1192 • Imugan

20856-57-9

Use	Fungicide.	
LC50 values to fishes, mg/l	3.7	96hr, Rasbora heteromorpha (Tooby et al. 1975)

1193 • Iodine

7553-56-2

LC50 values to fishes, mg/l	0.44	24hr, Ictalurus punctatus (LeValley 1982)

GHI

1194 • Ioxynil

1689-83-4

Synonyms	4-Hydroxy-3,5-diiodobenzonitrile 3,5-Diiodo-4-hydroxybenzonitrile 4-Cyano-2,6-diiodophenol Totril *
Sumformula of the chemical	C7H3I2NO
Products containing the chemical	Totril * ioxynil 225 g/l (PESREG)
Use	Active ingredient in herbicides.
State and appearance	Colourless/white crystalline solid. (PESREG)
Odour	Odourless.
Molecular weight	370.91
Vapour pressure, mmHg	0.0000047 at 25 °C (PESREG)
Water solubility, mg/l	50 at 25 °C (Pesticide Manual 1987)
Melting point, °C	209 (Pesticide Manual 1987) 212 with decomposition (PESREG)
Log octanol/water coefficient, log Pow	3.51 (PESREG)
Adsorption/desorption	Adsorption and desorption of ioxynil were studied with four soil types and the adsorption and desorption coefficients and constants were determined.

soil type	% org. carbon	adsorption Ka	adsorption Koc	desorption Kd	desorption Koc
peat	17.4	182	1046	166	954
clay	3.3	6	182	8	251
loam	1.9	5	276		
sand	1.4	4	250		

(PESREG)

Mobility	The leaching behaviour of (C-14) ioxynil (0.8 kg a.i./ha) was studied in four soil (sand, loam, peat and clay) columns. 0.02–0.45% of applied radioactivity was found in leachate water (230 ml/in different times) of sand, loam and clay soil columns and 1.1–3.0% in leachate water (247 ml/in different times) of aged loam (ageing 2 days) and sand (ageing 1 day) soil columns. (PESREG) Sublimes at 140 °C at 0.15 mm. (PESREG) Solubility in organic solvents (mg/100 ml): methanol: 2000 acetone: 7000 benzene: 500 (PESREG)

GHI

Aerobic degradation in soil	The degradation of ioxynil was studied under aerobic conditions (0.8 kg a.i./ha, 22 °C) on sand and loam soils. in the sand soil: *days after treatment* / *volatiles %* / *extractable %* / *non-extractable %* 1 / 0.4 / 86.6 / 10.9 3 / 2.0 / 63.1 / 33.9 7 / 10.5 / 30.6 / 57.1 48 / 27.3 / 8.7 / 72.5 in the loam soil: *days after treatment* / *volatiles %* / *extractable %* / *non-extractable %* 1 / 1.0 / 80.1 / 12.7 3 / 6.1 / 47.6 / 38.6 7 / 15.4 / 18.2 / 57.3 42 / 27.5 / 7.1 / 68.0 The major metabolites were 3,5-di-iodo-4-hydroxybenzamide and 3,5-di-iodo-4-hydroxybenzoic acid. (PESREG) The rate of degradation of ioxynil were studied in four soils under aerobic conditions (0.8 kg a.i./ha, 10 °C and 22 °C, incubated 63 days). *half-life (days)* *soil* / *total extractable radioactivity 10 °C* / *22 °C* / *ioxynil 10 °C* / *22 °C* sand / 8.5 / 3.5 / 3.5 / 1.5 loam / 7.5 / 2.5 / 6.5 / 2 clay / 10 / 3 / 7.5 / 2.5 peat / 150* / 23 / 75* / 15.5 *estimated results The major metabolites were 3,5-di-iodo-4-hydroxybenzamide and 3,5-di-iodo-4-hydroxybenzoic acid. (PESREG)
Degradation and transformation products	3,5-di-iodo-4-hydroxybenzamide; 3,5-di-iodo-4-hydroxybenzoic acid (PESREG)
Other information about degradation	COD:30 ppm, 50 g/l at maximum solubility at 25 °C. (PESREG)
LD50 values to mammals in oral exposure, mg/kg	140 orl-rat (PESREG)
LD50 values to mammals in non-oral exposure, mg/kg	1050 idr-rat (PESREG)
LC50 values to mammals in inhalation exposure, mg/m³	380 4hr, ihl-rat (PESREG)
LD50 values to birds in oral exposure, mg/kg	170 orl-brd, Phasianus colchicus (PESREG) 100 orl-brd, Coturnix japonica (PESREG)
Effects on invertebrates	LC50, 35 ppm, 7d and 14d, Eisenia foetida (PESREG)
Effects on plants	Treatment of Vicia faba and Pisum sativum root tip meristems with ioxynil of 0.000001 M reduced the rate of entry into mitosis (Rost et al. 1977).
EC50 values to algae, mg/l	24 96hr, grw ihb, Scenedesmus substicatus (PESREG)
LC50 values to crustaceans, mg/l	3.9 48hr, Daphnia magna, GLP (PESREG)
LC50 values to fishes, mg/l	3.3 48hr, Rasbora heteromorpha (Pesticide Manual 1983) 8.5 96hr, Salmo gairdneri, GLP (PESREG)

1195 • Iron and iron compounds 7439-89-6

Synonyms	Ferric ion Ferrous ion	
Effects on amphibia	LC50 (96hr) 17.62 mg/l, tadpoles of Rana hexadactyla (Khangarot et al. 1985).	
LC50 values to crustaceans, mg/l	5.9 9.6	21d, Daphnia magna 48hr, with food, D.magna (Biesinger & Christensen 1972)
	81.1	Fe(III), 48hr, Asellus aquaticus (Furmanska 1979)
	124 183	Fe(III), 96hr, Asellus aquaticus Fe(III), 48hr, Asellus aquaticus (Martin & Holdich 1986)
EC50 values to crustaceans, mg/l	5.2	21d, rpd, Daphnia magna (Biesinger & Christensen 1972)
LOEC values to crustaceans, mg/l	4.4	21d, rpd, Daphnia magna (Biesinger & Christenssen 1972)
LC50 values to fishes, mg/l	80 75 230	24hr, Alburnus alburnus 24hr, Platichthys flesus 24hr, Perca fluviatilis (Bagge & Ilus 1975)

1196 • Iron(III) oxide 1309-37-1

Synonyms	Anhydrous iron oxide Black oxide of iron Ferric oxide Ironoxide Red oxide of iron Yellow oxide of iron	
Sumformula of the chemical	Fe2O3	
Molecular weight	159.7	
LD50 values to mammals in non-oral exposure, mg/kg	5400 5500	ipr-mus ipr-rat (Sweet 1987)
LDLo values to mammals in non-oral exposure, mg/kg	30	scu-dog (Sweet 1987)
TDLo values to mammals in non-oral exposure, mg/kg	135	scu-rat, tumorigenic (Sweet 1987)

GHI

1197 • Iso-butanol 78-83-1

Synonyms	Isobutyl alcohol Isopropylcarbinol 2-Methyl-1-propanol 2-Methylpropyl alcohol 1-Hydroxymethylpropane 2-Methylpropan-1-ol
Sumformula of the chemical	C4H10O

Use	The major use of isobutanol is in the manufacture of isobutyl acetate, which is employed in the lacquer industry. Furthermore, isobutanol is used as a solvent in paint and varnish removers and in the manufacture of isobutyl esters, which serve as solvents, plasticizers, flavourings, and perfumes. It is also used as a flavouring agent in butter, cola, fruit, liquor, rum, and whisky (Hall & Oser 1965). Isobutanol is one of the three main alcohols in fused oil, and is present in large amounts in some alcoholic beverages (Hedlund Kiessling 1969). Natural isobutanol is produced by the fermentation of carbohydrates. Isobutanol is found in some fruits. It also occurs in beverages. Isobutanol has been identified in sundry other foods including cheddar cheese and hop oil (WHO 1987).
Restrictions to use	The Council of Europe (1981) included isobutanol in the list of flavouring substances that can be added to foodstuffs without hazard to public health at a level of 25 mg/kg for beverages and food (WHO 1987).
State and appearance	Colourless liquid.
Odour	Sweet, similar to that of amyl alcohol, but weaker. Odour threshold: approximately 4.6 mg/m^3 (1.5 ppm). Quality: sweet, musty Hedonic tone: unpleasant to pleasant Threshold odour concentration absolute: 0.68 ppm 50% recognition: 1.80 ppm 100% recognition: 2.05 ppm Odour index 100% recognition: 5 131 (Hellman & Small 1974).
Molecular weight	74.12
Density, kg/m^3	801–803
Conversion factor, 1 ppm in air=	3.083 mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.324 ppm
Boiling point, °C	108 760 mmHg (MITI 1992)
Log octanol/water coefficient, log Pow	0.76 (Sangster 1989)
Chemical oxygen demand, g 02/g	2.46 5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.41 5 days (Bridie et al. 1979)
Total degradation in water	Biodegradation: 90% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

Other information about degradation	Isobutanol is readily biodegradable. It is degraded in significant amounts within a few hours, and degradation would be expected to be complete within a few days (WHO 1987). Nazarenko (1969) reports an oxygen requirement of approximately 1.4 mg to oxidize 1 mg of isobutanol. In animals, isobutanol is absorbed through the skin, lungs, and gastrointestinal tract. Isobutanol is metabolized by alcohol dehydrogenase to isobutyric acid via the aldehyde and may enter the tricarboxylic acid cycle. Small amounts of isobutanol are excreted unchanged, ot as the glucoronide in the urine. In rabbits, metabolites found in the urine include acetaldehyde, acetic acid, isobutyraldehyde, and isovaleric acid.
Other information about bioaccumulation	Isobutanol does no bioaccumulate (Chiou et al. 1977).
LD50 values to mammals in oral exposure, mg/kg	2460 orl-rat 3500 orl-mus 3100 orl-rat (US DHEW 1078; Kushneva et al. 1983)
LD50 values to mammals in non-oral exposure, mg/kg	4240 skn-rbt (US DHEW 1978)
LC50 values to mammals in inhalation exposure, mg/m³	19900 ihl-gpg 15500 ihl-mus 26250 ihl-rbt 19200 ihl-rat (Kushneva et al.1983)
Effects on the physiology of mammals	The acute toxic effects are alcoholic intoxication and narcosis. Isobutanol is severely irritating to the eyes and moderately irritating to the skin. A group of rats given an 1 mol/l solution of isobutanol as their sole drinking liquid for 4 months did not show any adverse effects in the liver; another group given a 2 mol/l solution as their sole drinking liquid for 2 months showed a reduction in fat, glycogen, ant RNA content, and in the overall size of the cells in the liver. Continuous inhalation exposure of rats to 3 mg/m³ for 4 months resulted in depression of leg withdrawal response to electrical stimulation, minor changes of formed elements of the blood and serum enzymes. The estimated NOEC level was 0.1 mg/m³ (WHO 1987).
Carcinogenicity	In a lifetime carcinogenicity study, groups of rats received isobutanol subcutaneously (0.05 ml/kg body weight twice a week) or orally (0.2 mg/kg). The animals exhibited toxic liver damage ranging from steatosis to cirrhosis. Numbers of animals showing malignant tumours totalled 8 in the subcutaneous group, 3 in the oral group, and 0 in the control group. The majority of treated animals also showed hyperplasia of blood-forming tissues. Because of lack of mutagenicity studies, the Task Group could not determine whether isobutanol was a genetically active compound. The findings in the carcinogenicity study ar a cause of concern. Because of methodological inadequacies and the manner of reporting the data, it was not possible to determine whether isobutanol should be regarded as an animal carcinogen. Thus it is not possible to extrapolate from this study to possible long-term effects in man (WHO 1987).
Mutagenicity	No adequate data are available to assess mutagenicity of teratogenicity of isobutanol or effects on reproduction (WHO 1987).
Effects on amphibia	Threshold for narcosis: 4000 mg/l, Tadpole (Rana sp.), Münch (1972).
Effects on plants	Toxicity studies in plants indicate that germination will not be affected by exposure to isobutanol at background levels. An EC50 of 760 mg/l was reported by Reynolds (1977) for seed germination in lettuce (Lactuca sativa). Smith & Siegel (1975) found an EC50 of 40800 mg/l for seed germination in cucumber (Cucumis sativus).

Effects on microorganisms	Toxicity of isobutanol to microorganisms (WHO 1987).

Species	Conc. mg/l	Parameter	Reference
Protozoa			
Chilomonas paramaecium (flagellate)	22	NOEC 48hr total biomass	Bringmann & Kühn 1981
Uronema parduczi (ciliate)	169	NOEC 20hr total biomass	Bringmann & Kühn 1981
Entosiphon sulcatum (flagellate)	296	NOEC 72hr total biomass	Bringmann & Kühn 1981
Bacteria			
Pseudomonas putida	280	NOEC 16hr total biomass	Bringmann & Kühn 1981
Bacillus subtilis	1180	EC50 spore germination	Yasuda-Yasaki et al. 1978

Toxicity threshold (cell multiplication inhibition test):
bacteria (Pseudomonas putida): 280 mg/l (Bringmann & Kühn 1980a).

EC50 values to microorganism, mg/l	1224 Microtox (Nacci et al. 1986) 14602 Biodegradation inhibition (Vaishnav 1986)
NOEC values to algae, mg/l	350 8d, grw, Scenedesmus quadricauda 290 8d, grw, Microcystis aeruginosa (Bringmann & Kühn 1978a)
LC50 values to crustaceans, mg/l	1400 24hr, Artemia salina (Price et al.1974)
EC50 values to crustaceans, mg/l	1250 24hr, mbt, Daphnia magna (Bringmann & Kühn 1982) 3800 Artemia salina, excyctment (Smith & Siegel 1975)
LC50 values to fishes, mg/l	1520 48hr, Leuciscus idus melanotus (Juhnke & Lüdemann 1978) 2600 24hr, Carassius auratus (Bridie et al.1979) 1000–3000 96hr, Alburnus alburnus (Linden et al.1979)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 350 mg/l protozoa (Entosiphon sulcatum): 295 mg/l (Bringmann & Kühn 1980a)

1198 • Isoamyl salicylate 87-20-7

Sumformula of the chemical	C12H16O3
EINECS-number	2017304
Boiling point, °C	276–278 (MITI 1992)
Total degradation in water	Biodegradation: 83.4% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

GHI

1199 • Isobenzan

297-78-9

Other information about mammals	ALD = 12 mg/kg, act, orl, deer mouse; LDfr = 87.5 mg/kg, subacute, deer mouse (Virtanen & Nuuja 1987).
LD50 values to birds in oral exposure, mg/kg	3.16 orl-Agelaius phoeniceus 2.37 orl-Sturnus vulgaris 4.22 orl-Coturnix coturnix 1 orl-Passer domesticus 1.33 orl-Quiscalus quiscula 10 orl-Columba livia (Schafer et al. 1983)

1200 • Isobutylacetate

110-19-0

Use	Solvent.
Odour	Quality: sweet, ester Hedonic tone: pleasant Threshold odour concentration absolute: 0.35 ppm 50% recognition: 0.50 ppm 100% recognition: 0.50 ppm Odour index 100% recognition: 34 200 (Hellman & Small 1974).
Water solubility, mg/l	7500 20 °C
Boiling point, °C	117.2
Volatilization	Relative volatility (nBuAc=1) = 1.45
LD50 values to mammals in oral exposure, mg/kg	13000 orl-rat
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 200 mg/l (Bringmann & Kühn 1980a).
LOEC values to algae, mg/l	80 rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 80 mg/l protozoa (Entosiphon sulcatum): 411 mg/l (Bringmann & Kühn 1980a).

1201 • N-Isobutylmorpholine

10315-98-7

Sumformula of the chemical	C8H17ON
Water solubility, mg/l	28000 (MITI 1992)
Melting point, °C	< -10 (MITI 1992)
Boiling point, °C	180–182 (MITI 1992)
Log octanol/water coefficient, log Pow	1.02–1.32 (MITI 1992)
Total degradation in water	Biodegradation: 0–1% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

GHI

Bioconcentration factor, fishes	1.3–2.3 < 1.0	6w, Cyprinus carpio, conc 0.5 mg/l 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
LC50 values to fishes, mg/l	64.2	48hr, Oryzias latipes (MITI 1992)

1202 • Isobutyronitrile

78-82-0

Sumformula of the chemical	C4H7N	
EINECS-number	2011475	
Water solubility, mg/l	35	(20 °C) (MITI 1992)
Melting point, °C	-71.5	(MITI 1992)
Boiling point, °C	103.9	(MITI 1992)
Total degradation in water	Biodegradation: 53.9% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

1203 • Isocyanuric acid

108-80-5

Bioconcentration factor, fishes	< 0.1 < 0.5	6w, Cyprinus carpio, conc 10 mg/l 6w, Cyprinus carpio, conc 1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	> 1000	48hr, Oryzias latipes (MITI 1992)

1204 • Isodrin

465-73-6

LC50 values to fishes, mg/l	0.012 0.006	96hr, Lepomis macrochirus 96hr, Pimephales promelas (Khan et al. 1973)
Other information	Isodrin is isomere of aldrin.	

1205 • Isofenphos

25311-71-1

Use	Active ingredient in insecticides.	
LC50 values to fishes, mg/l	2	96hr, Carassius auratus (Pesticide Manual 1983)

1206 • Isooctanol

26952-21-6

Synonyms	Isooctyl alcohol	
Use	Solvent.	
Water solubility, mg/l	1000	20 °C
Boiling point, °C	186	

GHI

Volatilization	Relative volatility (nBuAc=1) = 0.016
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 63 mg/l (Bringmann & Kühn 1980a).
LOEC values to algae, mg/l	8.5 rpd, schr, Scenedesmus quadricauda (Bringman & Kühn 1980a) 8.5 rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 8.5 mg/l protozoa (Entosiphon sulcatum): 30 mg/l (Bringmann & Kühn 1980a)

1207 • Isophorone

78-59-1

Synonyms	1,5,5-Trimethyl-1-cyclohexen-3-one
Use	Solvent; intermediate.
Odour	Quality: sharp Hedonic tone: unpleasant to pleasant Threshold odour concentration absolute: 0.20 ppm 50% recognition: 0.54 ppm 100% recognition: 0.54 ppm Odour index 100% recognition: 2 444 (Hellman & Small 1974).
Molecular weight	138
Melting point, °C	-8.1 (MITI 1992)
Boiling point, °C	215.2 (MITI 1992)
Log octanol/water coefficient, log Pow	1.67 (Anon. 1988)
Henry's law constant, Pa x m³/mol	4.8 (Anon. 1988)
Mobility	Equilibrium distribution: *mass %* air 65.92 water 33.83 solid 0.25 (Anon. 1988).
Total degradation in water	Biodegradation: 1.5% by BOD period: 14d substance: 100mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	1.1–1.8 6w, Cyprinus carpio, conc 0.5 mg/l < 10 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
LC50 values to crustaceans, mg/l	120 48hr, Daphnia magna (LeBlanc 1980)
LC50 values to fishes, mg/l	145–255 96hr, grw, juv. Pimephales promelas (Cairns & Nebeker 1982) 220 96hr, Lepomis macrochirus (Buccafusco et al. 1981) 340 48hr, Oryzias latipes (MITI 1992)

GHI

LOEC values to fishes, mg/l	144	grw, juv., Cyprinodon variegatus (Ward & Parrish 1980)
	14	grw, juv., Pimephales promelas (Cairns & Nebeker 1982)
Other information about water organisms	EC50 (24hr), 420 mg/l, rpd, Tetrahymena pyriformis (Yoshioka et al. 1985).	

1208 • Isophtalic acid dimethyl ester 1459-93-4

Sumformula of the chemical	C10H10O4	
Water solubility, mg/l	290	(MITI 1992)
Melting point, °C	67–69	(MITI 1992)
Total degradation in water	Biodegradation: 94–102% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1991).	

1209 • Isophthalic acid 121-91-5

Melting point, °C	350	(MITI 1992)
Total degradation in water	Biodegradation: 77.7% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	

1210 • Isopimaric acid 5835-26-7

LC50 values to fishes, mg/l	0.22	96hr, Oncorhynchus kisutch (Anon. 1980)
	0.3	96hr, Oncorhynchus kisutch (Rogers et al. 1975)

1211 • Isoprene 78-79-5

Vapour pressure, mmHg	760	32.6 °C (MITI 1992)
Water solubility, mg/l	440	(MITI 1992)
Melting point, °C	-145.95	(MITI 1992)
Boiling point, °C	34.08	(MITI 1992)
Log octanol/water coefficient, log Pow	2.42	(MITI 1992)
Total degradation in water	2% by BOD period: 28d substance: 10.0 mg/l sludge: 2 mg/l (MITI 1992).	

GHI

Bioconcentration factor, fishes	5.0–14 5.6–20	6w, Cyprinus carpio, conc 0.05 mg/l 6w, Cyprinus carpio, conc 0.005 mg/l (MITI 1992)
LC50 values to fishes, mg/l	74 43 180 46.6	96hr, Pimephales promelas 96hr, Lepomis macrochirus 96hr, Carassius auratus (Cage 1970) 48hr, Oryzias latipes (MITI 1992)

1212 • Isopropanol

67-63-0

Synonyms	2-Propanol Isopropyl alcohol Dimethylcarbinol Propan-2-ol sec-Propyl alcohol	
Sumformula of the chemical	C3H8O	
Use	Solvent.	
Odour	Quality: sharp, musty Hedonic tone: unpleasant Threshold odour concentration absolute: 3.20 ppm 50% recognition: 7.50 ppm 100% recognition: 28.2 ppm Odour index 100% recognition: 1 539 (Hellman & Small 1974).	
Molecular weight	60.11	
Conversion factor, 1 ppm in air=	2.5	mg/m^3 (Verschueren 1983)
Conversion factor, 1 mg/m^3 in air=	0.408	ppm (Verschueren 1983)
Boiling point, °C	82.5	
Log octanol/water coefficient, log Pow	0.05	(Sangster 1989)
Henry's law constant, Pa x m^3/mol	1.131	calc. (Yaws et al. 1991)
Volatilization	Relative volatility (nBuAc=1) = 2.30	
Chemical oxygen demand, g O2/g	2.23	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g O2/g	1.19	5 days (Bridie et al. 1979)
LD50 values to mammals in oral exposure, mg/kg	4797 3600 5045	orl-dog orl-mus orl-rat (Sweet 1987)

LD50 values to mammals in non-oral exposure, mg/kg	2560 3444 4477 2735 667 1509 1088 1184 12800	ipr-gpg ipr-hms ipr-mus ipr-rat ipr-rbt ivn-mus ivn-rat ivn-rbt skn-rbt (Sweet 1987)
LDLo values to mammals in oral exposure, mg/kg	3570	orl-hmn (Sweet 1987)
LDLo values to mammals in non-oral exposure, mg/kg	1963 5120 6 6000	ivn-cat ivn-dog scu-mam scu-mus (Sweet 1987)
LCLo values to mammals in inhalation exposure, ppm	12800 12000	ihl-mus, 3hr, ihl-rat, 8hr (Sweet 1987) ihl-mus, 3hr, ihl-rat, 8hr (Sweet 1987)
TDLo values to mammals in oral exposure, mg/kg	11340 5040 20160 6480 223 14432	orl-rat, 45d preg. maternal effects orl-rat, 1-20d preg. effects on fertility orl-rat, 1-20d preg. effects on fertility orl-rat, effects on newborn orl-hmn orl-man (Sweet 1987)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 1050 mg/l (Bringmann & Kühn 1980a).	
EC50 values to microorganism, mg/l	30897	Biodegradation inhibition (Vaishnav 1986)
LOEC values to algae, mg/l	1000	rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to fishes, mg/l	7060 10400 > 5000	7 d, Poecilia reticulata (Könemann 1979) 96hr, Pimephales promelas (Veith et al. 1983) 24hr, Carassius auratus (Bridie et al. 1982)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 1800 mg/l protozoa (Entosiphon sulcatum): 4930 mg/l (Bringmann & Kühn 1980a)	

1213 • 4-Isopropenyl-chlorobenzene 1712-70-5

Sumformula of the chemical	C_9H_9Cl	
Water solubility, mg/l	4.2	(MITI 1992)
Melting point, °C	1.5	(MITI 1992)
Boiling point, °C	214.5	(MITI 1992)
Log octanol/water coefficient, log Pow	4.62	(MITI 1992)

Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	473–916 8w, Cyprinus carpio, conc 0.01 mg/l 437–948 8w, Cyprinus carpio, conc 0.001 mg/l (MITI 1992)
LC50 values to fishes, mg/l	2.34 48hr, Oryzias latipes (MITI 1992)

1214 • 2-Isopropoxyphenyl methylcarbamate 114-26-1

Synonyms	Propoxur Barygon 2-(1-Methylethoxy) phenol methylcarbamate Aprocarb
Sumformula of the chemical	C11H15NO3
Use	Active ingredient in insecticides.
State and appearance	White to tan crystalline solid.
Molecular weight	209.27
Water solubility, mg/l	2000
Melting point, °C	91
Total degradation in water	After 8 weeks 5% of original compound found (river water in a sealed glass jar) (Eichelberger & Lichtenberg 1971).
LD50 values to mammals in oral exposure, mg/kg	70 orl-rat 32 orl-mus (Lewis & Sweet 1984) 95–104 orl-rat (Anon. 1976)
LD50 values to mammals in non-oral exposure, mg/kg	800 skn-rat (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	4 orl-bwd 9.58 orl-dck 28 orl-qal (Lewis & Sweet 1984) 3.83 orl-Agelaius phoeniceus 13.3–17.0 orl-Sturnus vulgaris 42.2 orl-Coturnix coturnix 13.3–15.0 orl-Passer domesticus 13.3 orl-Quiscalus quiscula 7.5 orl-Columba livia 4.22–10.0 orl-Carbodacus mexicanus 17.8 orl-Anas platyrhynchos 13.3–15.0 orl-Phasianus colchicus 7.5 orl-Xanthocephalus xanthocephalus 10 orl-Molothrus ater 13.3 orl-Corvus brachyrhynchos 5.62 orl-Cassidix major 17.8 orl-Zenaida macroura 4.22 Melopsittacus undulatus (Schafer et al. 1983)

GHI

Effects on arthropods	Pteronarcys californica: LC50 96hr, 0.013 mg/l (Sanders & Cope 1968). Fourth instar larval Chironomus riparius; LC50 24hr, 64.4 ppb (Estenik & Collins 1979).	
EC50 values to algae, mg/l	0.01	20hr, Dunaliella euchlora (Derby & Ruber 1971)
LC50 values to crustaceans, mg/l	0.011	Daphnia pulex (Nishiuchi & Hashimoto 1967)
	0.034	96hr, Gammarus lacustris (Sanders 1969)
	0.05	96hr, Gammarus fasciatus (Sanders 1972)
	0.37	act, Daphnia pulex (Hashimoto & Nishiuchi 1981)
	4.47 1.26	24hr, Daphnia magna 48hr, Daphnia magna (Bogacka & Groba 1980)
NOEC values to crustaceans, mg/l	0.4	rpd, schr, Daphnia magna (Macek & Sleight 1977)
LC50 values to fishes, mg/l	6.6 4–14	96hr, Lepomis macrochirus 96hr, Salmo gairdneri (Pesticide Manual 1983)
	2 1.4	48hr, Lebistes reticulatus 96hr, Lebistes reticulatus (Bogacka & Groba 1980)
	6 11.2	24hr, Salmo salar 24hr, Salmo trutta m. lacustris (Colquhoun & Dean 1980)
	5.2	96hr, Heteropneustes fossilis (Srivastava & Singh 1982)
	> 10 > 10	48hr, Cyprinus carpio 48hr, Carassius auratus (Hashimoto & Nishiuchi 1981)
	> 10	48hr, Cyprinus carpio (Nishiuchi & Hashimoto 1967)
NOEC values to fishes, mg/l	0.4	rpd, chr, Pimephales promelas (Macek & Sleight 1977)
Other information about water organisms	Dunaliella euchlora: 1000 ppb: 25% reduction in 02 evolution 100 ppb: 32% reduction in 02 evolution 10 ppb: 27% reduction in 02 evolution Phaeodactylum tricornutum: 1000 ppb: 23% reduction in 02 evolution 100 ppb: 28% reduction in 02 evolution 10 ppb: 40% reduction in 02 evolution Skeletonema costatum: 1000 ppb: 30% reduction in 02 evolution 100 ppb: 23% reduction in 02 evolution 10 ppb: 29% reduction in 02 evolution Cyclotella nana: 1000 ppb: 53% reduction in 02 evolution 02 evolution measured by Winkler Bottle technique; 1 l of culture incubated 20 hours in pesticide solution, then placed in test bottles 4 hours (Derby & Ruber 1971).	

GHI

1215 • Isopropyl benzyl alcohol 536-60-7

Boiling point, °C	246 (MITI 1992)
Total degradation in water	Biodegradation: 77.2–92.0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

1216 • 2-Isopropyl-4-methyl-6-hydroxypyrimidine 2814-20-2

Sumformula of the chemical	C8H12N20
Water solubility, mg/l	20000 (MITI 1992)
Melting point, °C	172–173.9 (MITI 1992)
Log octanol/water coefficient, log Pow	0.55 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.1–0.5 6w, Cyprinus carpio, conc 2 mg/l < 1.4–2.2 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	> 1000 48hr, Oryzias latipes (MITI 1992)

1217 • 1-Isopropyl-4-methylcyclohexane 99-82-1

Sumformula of the chemical	C10H20
EINECS-number	2027904
Water solubility, mg/l	0.28 (MITI 1992)
Melting point, °C	< -30 (MITI 1992)
Boiling point, °C	167–168.5 (MITI 1992)
Log octanol/water coefficient, log Pow	5.56 (MITI 1992)
Total degradation in water	Biodegradation: 57–95% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

GHI

1218 • Isopropyl-N-phenylcarbamate 122-42-9

Use	Pesticide.	
Log soil sorption coefficient, log Kom	1.71	(Sabljic 1987)
LC50 values to crustaceans, mg/l	10 10 10	96hr, Gammarus lacustris (Sanders 1969) 48hr, Daphnia pulex (Sanders & Cope 1966) Simocephalus serrulatus (Sanders & Cope 1966)

1219 • Isopropylacetate 108-21-4

Use	Solvent.	
Odour	Quality: sweet, ester Hedonic tone: pleasant to unpleasant Threshold odour concentration absolute: 0.49 ppm 50% recognition: 0.90 ppm 100% recognition: 0.97 ppm Odour index 100% recognition: 56 907 (Hellman & Small 1974).	
Boiling point, °C	90	
LD50 values to mammals in oral exposure, mg/kg	3000	orl-rat
LOEC values to algae, mg/l	165	rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a)

GHI

1220 • Isopropylamine 75-31-0

Synonyms	2-Aminopropane	
Sumformula of the chemical	C3H9N	
Odour	Quality: ammoniacal, amine Hedonic tone: unpleasant to pleasant Threshold odour concentration absolute: 0.21 ppm 50% recognition: 0.71 ppm 100% recognition: 0.95 ppm Odour index 100% recognition: 661 052 (Hellman & Small 1974).	
pKa	10.63	(Sangster 1989)
Log octanol/water coefficient, log Pow	0.26	(Sangster 1989)

1221 • Isopropylbenzene 98-82-8

Synonyms	Cumene 2-Phenylpropane

Odour	Quality: sharp Hedonic tone: pleasant Threshold odour concentration absolute: 0.008 ppm 50% recognition: 0.047 ppm 100% recognition: 0.047 ppm Odour index 100% recognition: 83 000 (Hellman & Small 1974).	
Boiling point, °C	145.2	
Log octanol/water coefficient, log Pow	3.66 3.66	(Anon. 1986) (Sangster 1989)
Henry's law constant, Pa x m³/mol	1469	calc. (Yaws et al. 1991)
Volatilization	Relative volatility (nBuAc=1) = 0.52	
Total degradation in water	Confirmed to be biodegradable (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	1400	
LD50 values to birds in oral exposure, mg/kg	> 98	orl-Agelaius phoeniceus (Schafer et al. 1983)

1222 • 4-Isopropylbenzoic acid 536-66-3

Sumformula of the chemical	C10H12O2	
Water solubility, mg/l	150	(MITI 1992)
Melting point, °C	116–120	(MITI 1992)
Total degradation in water	Biodegradation: 86–91% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

1223 • Isopropylbromide 75-26-3

Sumformula of the chemical	C3H7Br	
EINECS-number	2008551	
Melting point, °C	-89	(MITI 1992)
Boiling point, °C	59.4	(MITI 1992)
Total degradation in water	Biodegradation: 73–89% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

1224 • Isopropyldecalin 29690-50-9

Water solubility, mg/l	< 10	(MITI 1992)
Boiling point, °C	247–252	(MITI 1992)

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Log octanol/water coefficient, log Pow	6.19 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	1.670–7.780 8w, Cyprinus carpio, conc 0.1 mg/l 1.200–5.410 8w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be accumulated on a medium level (Anon. 1987).
LC50 values to fishes, mg/l	6.5 48hr, Oryzias latipes (MITI 1992)

1225 • Isopropylnaphthalene 29253-36-9

Water solubility, mg/l	0.55 (MITI 1992)
Boiling point, °C	266.5 (MITI 1992)
Log octanol/water coefficient, log Pow	5.11 (MITI 1992)
Total degradation in water	Biodegradation: 0–24% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).
Bioconcentration factor, fishes	492–2750 8w, Cyprinus carpio, conc 0.05 mg/l 220–980 8w, Cyprinus carpio, conc 0.005 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be accumulated on a medium level (Anon. 1987).
LC50 values to fishes, mg/l	1.55 48hr, Oryzias latipes (MITI 1992)

1226 • Isoprotiolane 50512-35-1

EC50 values to algae, mg/l	3.4 grw, Chlamydomonas reinhardii (Lee & Hong 1982)

1227 • Isoproturon 34123-59-6

Use	Herbicide.
Effects on plants	0.125 kg a.i. isoproturon/ha was applied with a sprayer to blackgrass (Alopecurus myosuroides Huds.) at the 2 to 3-leaf stage —a decrease in mean fresh weight of plants (Blair 1978).

1228 • Juvabiol 60134-56-7

LC50 values to fishes, mg/l	2 96hr, Salmo gairdneri (Leach et al. 1975)

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1229 • Juvabione 17904-27-7

LC50 values to fishes, mg/l	1.5	96hr, Salmo gairdneri (Leach et al. 1975)

1230 • Kanechlor 500 37317-41-2

Effects on the physiology of water organisms	Cyprinus carpio, 250 mg/kg, change in enzyme activity (Yamashita et al. 1987). Salmo gairdneri, 500 mg/kg, 6 d, biochemical effect (change in physiochemical process including glycogen uptake, cholesterol levels and lipis analysis) (Miyauchi & Uematsu 1987).

1231 • Karbutilate 4849-32-5

Synonyms	tert-Butylcarbamic acid ester with 3(m-hydroxyphenyl)-1,1-dimethylurea
Use	Herbicide.
Effects on plants	1.75 kg karbutilate/ha was applied with a sprayer (preemergence) following seeding to lamb's-quarters (Chenopodium album L.) → plants (seeds) were killed (Jensen et al. 1977).

1232 • Kasugamycin 6980-18-3

Use	Fungicide.	
LC50 values to crustaceans, mg/l	> 40	act, Daphnia pulex (Hashimoto & Nishiuchi 1981)
	> 40	act, water flea (Pesticide Manual 1983)
LC50 values to fishes, mg/l	> 40	act, Cyprinus carpio
	> 40	act, Carassius auratus (Pesticide Manual 1983)
	> 40	act, Cyprinus carpio
	> 40	act, Carassius auratus (Hashimoto & Nishiuchi 1981)

1233 • Kepone 143-50-0

Synonyms	1,3,4-Metheno-2H-cyclobuta(cd)pentalen-2-one, 1,1a,3,3a,4,5,5,5a,5b,6-decachloroctahydro- Decachlorooctahydro-1,3,4-metheno-2H-cyclobuta(cd)pentalen-2-one Decachlorotetrahydro-4,7-methanoindeneone Chlordecone Merex
Sumformula of the chemical	C10Cl100
Use	Pesticide (ants, cockroaches). Used also in banana plantations.
State and appearance	Highly stable odourless colourless solid.
Odour	Odourless.
Molecular weight	490.6
Vapour pressure, mmHg	0.0000003
Water solubility, mg/l	7.6 24 °C
Total degradation in soil	Disappearance after 5 months in soil is minimal (Verschueren 1983).

JKL

Bioconcentration factor, fishes	1211–1548 (Verschueren 1983)
Bioconcentration factor, crustaceans	8.1–698 (Verschueren 1983)
Bioconcentration factor, algae	230–800 (Verschueren 1983)
LD50 values to mammals in oral exposure, mg/kg	95 orl-rat (Lewis & Sweet 1984) 65 orl-rbt (Verschueren 1983) 250 orl-dog (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	345 skn-rbt 126 unk-mam (Lewis & Sweet 1984) 100–150 ukn-rat (Virtanen & Nuuja 1987)
TDLo values to mammals in oral exposure, mg/kg	16.5 orl-mus, fertility 63 orl-rat, effects on newborn (Lewis 1987) 200 orl-rat 1200 orl-mus (Lewis & Sweet 1984)
TDLo values to mammals in non-oral exposure, mg/kg	50 rat-ipr, maternal effects 2 rat-scu, maternal effects 10 rat-scu, maternal effects (Lewis 1987)
Effects on the physiology of mammals	Neuro- and livertoxic (Virtanen & Nuuja 1987).
Other information about mammals	LDfr = 100 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987) (chlordecone).
Carcinogenicity	Carcinogenic by RTECS criteria (Sweet 1987). Carcinogenic determination; animal positive, human suspected. NCI carcinogenesis bioassay completed; results positive; mouse, rat (Lewis & Sweet 1984).
LD50 values to birds in oral exposure, mg/kg	480 orl-ckn 237 orl-qal (Lewis & Sweet 1984) 237–316 orl-Coturnix coturnix (Schafer et al. 1983)
EC50 values to algae, mg/l	0.35 rpd, schr, 7 d, Chlorococcum sp. (Walsh et al. 1977) 0.58 rpd, schr, 7 d, Dunaliella terticulata (Walsh et al. 1977)
EC50 values to crustaceans, mg/l	0.12–0.67 srv, act,48hr, Daphnia magna (Barera & Adams 1983)
LC50 values to fishes, mg/l	0.0066 96hr, Leistomus canthurus 0.065 96hr, Cyprinodon variegatus (Hansen et al. 1977) 0.34 96hr, Pimephales promelas (Buckler et al. 1981) 0.036 96hr, Salmo gairdneri 0.02 96hr, Salmo trutta (deWitt & George 1959) 0.035 96hr, Anguilla rostrata 0.05 96hr, Lepomis macrochirus 0.514 96hr, Ictalurus punctatus (Roberts & Bendl 1982) 0.138 4d, Fundulus heteroclitus (Rice & Mills 1987)

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LOEC values to fishes, mg/l	0.00008 srv, grw, schr, Cyprinodon variegetus (Hansen et al. 1972) 0.00012 grw, chr, Cyprinodon variegatus (Hansen et al. 1972) 0.003 srv, chr, Pimephales promelas (Buckler et al. 1981) 0.0008 srv, schr, 28 d, Cyprinodon variegatus (Hansen et al. 1977)
NOEC values to fishes, mg/l	0.00007 grw, chr, Cyprinodon variegatus (Hansen et al. 1972) 0.001 grw, Pimephales promelas (Buckler et al. 1981)
Effects on the physiology of water organisms	Fundulus heteroclitus, 0.050 mg/l, 10 d, change in enzyme activity (Rice & Mills 1987).

1234 • Kitazin

26087-47-8

LC50 values to fishes, mg/l	3.7 24hr, Cyprinus carpio (Hashimoto et al. 1982)

1235 • Lactonitrile

78-97-7

Synonyms	2-Hydroxypropionitrile
Sumformula of the chemical	C3H5NO
Molecular weight	71.09
LD50 values to mammals in oral exposure, mg/kg	87 orl-rat (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	15 ipr-mus (Sweet 1987)
LDLo values to mammals in non-oral exposure, mg/kg	5.2 scu-rbt 20 skn-rbt (Sweet 1987)
LCLo values to mammals in inhalation exposure, ppm	125 ihl-rat, 4hr (Sweet 1987)
Effects on amphibia	Frog, subcutaneous, LDLo 200 mg/kg (Sweet 1987).
LC50 values to fishes, mg/l	0.215 24hr, pinperch (Garret & Dougherty 1951) 0.9 96hr, Pimephales promelas 1.37 96hr, Poecilia reticulata (Jones 1971)

1236 • Landrine

12407-86-2

Other information about water organisms	LC50 (24hr), 0.051 mg/l, Chironomus riparius (Estenik & Collins 1979).

1237 • Lanthanum and lanthanum compounds

7439-91-0

LC50 values to fishes, mg/l	0.02 28d, Salmo gairdneri (Birge et al. 1980)

1238 • Larvin

59669-26-0

Synonyms	Bismethomyl thioester Bis-(O-(1-methyl-thioethylimino)-N-methylcarbamicacid)-N,N'-sulfide

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EC50 values to algae, mg/l	0.366–0.547 rpd, 96hr, Skeletonema costatum (Borthwick & Walsh 1981)
LC50 values to crustaceans, mg/l	0.263 96hr, Mysidopsis bahia (Borthwick & Walsh 1981)

1239 • Lauryl dimethyl amine 112-18-5

Synonyms	Dimethyldodecylamine
Total degradation in water	Biodegradation: 49.4% by BOD (on the upward trend) period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
LD50 values to birds in oral exposure, mg/kg	> 101 orl-Agelaius phoeniceus (Schafer et al. 1983)

1240 • Lauryllactam 947-04-6

Sumformula of the chemical	C12H23NO
Water solubility, mg/l	290 (MITI 1992)
Melting point, °C	149–151 (MITI 1992)
Log octanol/water coefficient, log Pow	2.92 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	0.8–1.2 6w, Cyprinus carpio, conc 0.5 mg/l < 2.6 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
LC50 values to fishes, mg/l	68.4 48hr, Oryzias latipes (MITI 1992)

1241 • N-Layroyl sarcosine sodium salt 137-16-6

Synonyms	Glycine, N-methyl-N-(1-oxododecyl)-, sodium salt
Sumformula of the chemical	C15H29NO3.Na
EINECS-number	2052815
Total degradation in water	Biodegradation: 86% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

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1242 • Lead acetate 301-04-2

Sumformula of the chemical	Pb(C2H302)2 . 3H20	
Use	Dyeing of textiles, waterproofing, varnishes, lead driers, chrome pigments, gold cyanidation process, insecticide, antifouling paints, analytical reagent, hair dye.	
State and appearance	White crystals of flakes (commercial grades are frequently brown or gray lumps).	
Odour	Sweetish taste.	
Molecular weight	325.29	
Melting point, °C	75	loses water
Boiling point, °C	280	anhydrous
Degradation point, °C	200	
Other physico–chemical properties	Adsorbs carbon dioxide when exposed to air, becoming insoluble in water. Soluble in water, slightly soluble in alcohol, freely soluble in glycerol. Combustible (Sax & Lewis 1987).	
LDLo values to mammals in oral exposure, mg/kg	300	orl-dog (Lewis & Sweet 1984)
Health effects	Toxic by ingestion, inhalation, and skin absorption(Sax & Lewis 1987).	
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 1.8 mg/l (Bringmann & Kühn 1980a)	
LOEC values to algae, mg/l	0.45	rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to crustaceans, mg/l	5 2.69	1d, Daphnia magna 2d, Daphnia magna (Khangarot et al. 1987)
EC50 values to crustaceans, mg/l	4.89 3.61	mbt, 1d, Daphnia magna mbt, 2d, Daphnia magna (Khangarot & Ray 1987)
LC50 values to fishes, mg/l	43.6	96hr, Pimephales promelas (Curtis & Ward 1981)
Effects on the physiology of water organisms	Delayed cytogenetic effect in recovery water, 1 d, 0.060 mg/l (data recalculation to ion concentration) (Sharma et al. 1988). Barytelphusa guerini (data recalculation to ion concentration): 1 d, 0.300 mg/l, hematological effect; 1–30 d, 0.300 mg/l, physiological effect (Tulasi & Rao 1988a, b).	
Other information about water organisms	LOEC 0.07 mg/l, rpd, schr, Uronema parduczi (Bringmann & Kühn 1980b). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 3.7 mg/l protozoa (Entosiphon sulcatum): 0.02 mg/l (Bringmann & Kühn 1980a)	

1243 • Lead and lead compounds 7439-92-1

Sumformula of the chemical	Pb
Use	Accumulator manufacturing; antiknock combounds for gasoline; brass manufacturing; cable mantles; anticorrosive pigment (red lead; chrome yellow; white lead); organic lead compounds (additive in colours).
Molecular weight	207.19

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Mobility	Relatively unsoluble lead sulfate, lead phosphate and lead carbonate is formed in soil. Adsorption to clay minerals, Fe- and Mn-oxides decreases also mobility of Pb. In acid soils Pb is strongly complexed with organic material (Kabata-Pendias & Pendias 1984). In water environment Pb is mainly complexed or adsorbed to particular material and sediment (Kabata-Pendias & Pendias 1984).	
Other information about metabolism	Pb is excreted via urine and feces (Grandjean & Nielsen 1979).	
TDLo values to mammals in oral exposure, mg/kg	450	6yr, orl-wmn (Lewis & Sweet 1984)
TCLo values to mammals in inhalation exposure, mg/kg	0.01	ihl-hmn (Lewis & Sweet 1984)
Effects on the physiology of mammals	Rats exposed to 0.011 mg inorganic Pb/m^3 in air for 6 hours per day for 3 months showed changes in behaviour (Waldron & Stöfen 1974).	
Health effects	Inhibition of growth, disorders in nervous system, impaired resistence to infections; genetic damages etc. in mammals (Folkesson 1976).	
Carcinogenicity	Chronic lead poisoning can cause tumours in kidneys (Waldron & Stöfen 1974).	
LDLo values to birds in oral exposure, mg/kg	160	orl-pgn (Lewis & Sweet 1984)
Effects on amphibia	LC50 (96hr), 33.28 ppm, tadpoles of Rana hexadactyla (Khangarot et al. 1985).	
Effects on plants	18.8 mg Pb/kg of dry matter (upper critical tissue concentration for sitka-spruce (Picea sitchensis) seedlings; concentration above which yields are reduced because of toxic effects (Burton et al. 1983). Diethyllead dichloride: 0.0000001 mol/l, 24hr, Spindle disturbances; Triethyllead chloride : 0.0000001 mol/l, 6hr, mitotic changes; Dimethyllead dichloride: 0.0000001 mol/l, 24hr index (Allium cepa); Trimethyllead chloride: 0.000001 mol/l, 6hr (Ahlberg et al. 1972) Lead nitrate: 10–4 mol/l, 6hr Young plantlets of lettuce (Lactuva sativa) were influenced by tetramethyl lead in the form of water solutions (0.001%) for 0–24 hours –in the rootcells following organels are damaged; the nucleus, the mitochondria, the Golgi apparatus, the endoplasmic reticulum and the proplastids; disturbances of cell division (Sekerka & Bobak 1974).	
EC50 values to algae, mg/l	0.14	rpd, schr, Selenastrum capricornutum (Christensen et al. 1979)
	11	96hr, rpd, Navicula incerta (Rachlin et al. 1983)
LC50 values to crustaceans, mg/l	0.3	21d, Daphnia magna
	0.45	48hr, with food, D.magna (Biesinger & Christensen 1972)
	64.1	96hr, mbt, Asellus aquaticus
	120	48hr, mbt, Asellus aquaticus (Martin & Holdich 1986)
EC50 values to crustaceans, mg/l	0.1	21d, rpd, Daphnia magna (Biesinger & Christensen 1972)
LOEC values to crustaceans, mg/l	0.03	rpd, 21d, Daphnia magna (Biesinger & Christensen 1972)
LC50 values to fishes, mg/l	0.22	28d, Salmo gairdneri (Birge et al. 1980)
	26	96hr, Colisa fasciata (Saxena & Parashari 1983)
	19	96hr, Channa punctata (Srivastava & Mishra 1979)

LOEC values to fishes, mg/l	0.0007	srv, chr, Salmo gairdneri
	0.032	rpd, grw, chr, Salmo gairdneri (Davies et al. 1976)
	0.084	srv, grw, chr, Salvelinus fontinalis (Holcombe et al. 1976)
	0.062	rpd, chr, Platichthys flesus (McKim 1977)
NOEC values to fishes, mg/l	0.0004	srv, chr, Salmo gairdneri
	0.018	rpd, grw, chr, Salmo gairdneri (Davies et al. 1976)
	0.039	srv, grw, chr, Salvelinus fontinalis (Holcombe et al. 1976)
	0.031	rpd, chr, Platichthys flesus (McKim 1977)

1244 • Lead carbonate

598-63-0 * CH2O3 Pb

1319-46-6 * C2H2O8 Pb3

Synonyms	Lead carbonate, basic Lead subcarbonate White lead Lead flake
Use	Exterior paint pigment; ceramic glazes.
State and appearance	White amorphous powder.
Degradation point, °C	400
Other physicochemical properties	Soluble in acids, insoluble in water; noncombustible (Sax & Lewis 1987).
Health effects	Toxic by inhalation (Sax & Lewis 1987).
LC50 values to fishes, mg/l	110 7d, Carassius auratus (Kemp et al. 1973)

1245 • Lead chloride

7758-95-4

Sumformula of the chemical	PbCl2
Use	Preparation of lead salts, lead chromate pigments, analytical reagent.
State and appearance	White crystals.
Melting point, °C	498
Boiling point, °C	950
Other physicochemical properties	Slightly soluble in hot water, insoluble in alcohol and cold water; noncombustible (Sax & Lewis 1987).
Health effects	Toxic by inhalation (Sax & Lewis 1987).
EC50 values to algae, mg/l	2.7 0.17d, Scenedesmus quadricauda pht (Starodub et al. 1987b)
LC50 values to crustaceans, mg/l	0.45 Pb, 48hr, Daphnia (Biesinger & Christensen 1972)
Effects on the physiology of water organisms	Nostoc muscorum, 0.02 d, 20.0 mg/l, photosynthesis effect (Rai & Raizada 1988). Scenedesmus quadricauda, 15 d, 1.0–3.0 mg/l, change in cell number of algae species (Starodub et al. 1987b).
Other information about water organisms	Poteriochromonas malhamensis, 258.8 mg/l, 3 d, 100% mortality including algicidal and herbicidal effects (Roderer 1987).

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1246 • Lead nitrate 10099-74-8

Sumformula of the chemical	Pb(NO3)2
Use	Lead salts, mordant in dyeing and printing calico, matches, mordant for staining mother-of-pearl, oxidizer in the dye industry, sensitizer in photography, explosives, tanning, process engraving, and lithography.
State and appearance	White crystals.
Degradation point, °C	470
Other physicochemical properties	Soluble in water and alcohol. Strong oxidizing material, dangerous fire risk in contact with organic materials (Sax & Lewis 1987).
EC50 values to crustaceans, mg/l	120 mbt, 2d, Asellus aquaticus 64.1 mbt, 4d, Asellus aquaticus 43.8 mbt, 2d, Crangonyx pseudogracilis 27.6 mbt, 4d, Crangonyx pseudogracilis (Martin & Holdich 1986)
LC50 values to fishes, mg/l	13.2 96hr, Channa punctata 12 96hr, Heteropneustes fossilis (Sastry & Gupta 1980) 6.6 7d, Carassius auratus (Kemp et al. 1973) 470 total Pb, 96hr, Salmo gairdneri 1.47 dissolved Pb, 96hr, Salmo gairdneri (Davies et al. 1976) 1625–1632 4d, Poecilia reticulata (Sehgal & Saxena 1987)
Effects on the physiology of water organisms	Barbus conchonius, 0.0474 mg/l, 30 d, biochemical effect (change in physiochemical process including glycogen uptake, cholesterol levels and lipis analysis) (Tewari et al. 1987). Colisa fasciata, 9.5 mg/l, 4 d, histological effect (presence of physical damage to tissues) (Srivastava 1987). (Data recalculation to ion concentration:) Barytelphusa guerini, 1 d, 0.300 mg/l, hematological effect; Barytelphusa guerini, 1–30 d, 0.300 mg/l, physiological effect (Tulasi & Rao 1988a, b); Chironomus plumosus, 0.08 d, 6.0 mg/l, oxygen consumption effect (Malyarevskaya & Karasina 1987); Clarias batrachus, 270 d, 3.0 mg/l, histological effect (Katti & Sathyanesan 1987a); Clarias batrachus, 150 d, 3.0 mg/l, physiological effect (Katti & Sathyanesan 1987b); Coretus corneus, 0.08 d, 6.0 mg/l, oxygen consumption effect; Pontogammarus maeoticus, 1 d, 60.0 mg/l, mortality; Pontogammarus maeoticus, 0.08 d, 0.6 mg/l, oxygen consumption effect (Malyarevskaya & Karasina 1987). Procambarus clarkii, 4 d, 400 mg/l, delayed oxygen consumption effect in recovery water (Torreblanca et al. 1987).
Other information about water organisms	Chara vulgaris, 0.0000075 M, 7 d, 100% mortality including algicidal and herbicidal effects (Heumann 1987). Carassius auratus, impaired efficiency, 0.07 mg Pb/l (Weir & Hime 1970).

1247 • Lead stearate 7428-48-0

Sumformula of the chemical	C18H3602.xPb
Use	Varnish and lacquer drier, high-pressure lubricants, lubricant in extrusion processes, stabilizer for vinyl polymers, corrosion inhibitor for petroleum, component of greases, waxes, and paints.
State and appearance	White powder.
Melting point, °C	107 (MITI 1992)

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Other physicochemical properties	Soluble in hot alcohol, insoluble in water. Combustible (Sax & Lewis 1987).
Total degradation in water	Biodegradation: 33% by BOD (on the upward trend) period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
Health effects	Toxic material. Absorbed by skin (Sax & Lewis 1987).

1248 • Lead tetroxide

1314-41-6

Synonyms	Lead orthoplumbate Lead oxide Lead tetraoxide Mineral orange Mineral red Trilead tetroxide Red lead oxide
Sumformula of the chemical	O4Pb3
Use	Storage batteries, glass, pottery and enameling, varnish, purification of alcohol, packing pipe joints, metal-protective paints, fluxes and ceramic glazes.
State and appearance	Bright red powder.
Molecular weight	685.57
Degradation point, °C	500–530
Other physicochemical properties	Partly soluble in acid, insoluble in water. An oxidising agent, may react with reducing agents. Toxic as dust (Sax & Lewis 1987).
LD50 values to mammals in non-oral exposure, mg/kg	220 ipr-gpg 630 ipr-rat (Sweet 1987)
LDLo values to mammals in oral exposure, mg/kg	1000 orl-gpg (Sweet 1987)
LD50 values to birds in oral exposure, mg/kg	> 111 orl-Agelaius phoeniceus (Schafer et al. 1983)

1249 • Lenacil

2164-08-1

Synonyms	3-Cyclohexyl-1,5,6,7-tetrahydrocyclopentapyrimidine-2,4-(3H)-dione 3-Cyclohexyl-6,7-dihydro-1H-cyclopentapyrimidine-2,4(3H,5H)-dione 3-Cyclohexyl-5,6-trimethyleneuracil Venzar *
Sumformula of the chemical	C13H18N2O2
Products containing the chemical	Venzar * lenacil 800 g/kg (PESREG)
Use	Active ingredient in herbicides.
State and appearance	White, crystalline solid. Wettable powder (Venzar *) (PESREG)

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Odour	Odourless. (PESREG)
Molecular weight	243.3
Water solubility, mg/l	6 at 25 °C (PESREG)
Melting point, °C	315.5–316.8 °C (PESREG)
Log octanol/water coefficient, log Pow	2.30–2.31 (PESREG)
Mobility	The leaching behaviour of (C-14) lenacil was studied in the soil columns. % of the applied radioactivity percolated through the columns in 50 cm of water: *sandy loam soil* *silty loam soil* freshly treated soil 86 0.52 aged (30 days) soil 9.3 1.0 (PESREG) Rf-values of lenacil on soil plates were 0.46 (sandy loam), 0.41 (sand) and 0.21–0.37 (silt loam). (PESREG) Solubility in organic solvents (g/100 g) at 25 °C: dimethylformamide: 0.8 buthylacetate: 0.4 cyclohexanone: 0.4 xylene: 0.2 (PESREG)
Photochemical degradation in water	Aqueous solutions of (C-14) lenacil were irradiated with simulated sunlight in a photo-reactor. About 85–90% was still present after an irradiation period of 30 days. (PESREG)
Hydrolysis in acid	The half-life of lenacil (6 ppm) was > 169 hours at pH 2. (PESREG)
Hydrolysis in base	The half-life of lenacil (6 ppm) was > 169 hours at pH 12. (PESREG)
Aerobic degradation in soil	Approximately 50% of 2-(C-14)-lenacil (2.3 ppm and 11.5 ppm) degraded to 14CO2 within 12 months under aerobic (silt loam soil) conditions. The half-life of intact (C-14) lenacil was to be approximately 3 months, and degradation was shown to be induced by microorganisms, since minimal 14CO2 production was observed in the sterile soil systems. Three metabolites 3-cyclohexyl-6,7-dihydro-7hydroxy-1H-cyclopentapyrimidine-2,4 (3H,5H)-dione, 3-cyclohexyl-5,6-dihydro-7H-cyclopentapyrimidine-2,4,7(1H,3H)- trione and 6,7-dihydro-3-(4-hydrocyclohexyl)-5H-cyclopenta(D)pyrimidine-2,4 (1H,3H)-dione. (PESREG)
Degradation and transformation products	3-cyclohexyl-6,7-dihydro-7hydroxy-1H-cyclopentapyrimidine-2,4 (3H,5H)-dione; 3-cyclohexyl-5,6-dihydro-7H-cyclopentapyrimidine-2,4,7(1H,3H)- trione; 6,7-dihydro-3-(4-hydrocyclohexyl)-5H-cyclopenta(D)pyrimidine-2,4 (1H,3H)-dione. (PESREG)
LD50 values to mammals in oral exposure, mg/kg	> 4000 orl-gpg male (PESREG)
LD50 values to mammals in non-oral exposure, mg/kg	> 5000 idr-rat albino (PESREG)
LC50 values to mammals in inhalation exposure, mg/m³	> 5.2 1hr, ihl-rat male (PESREG)
Subacute LC50 values to birds in feeding exposure, mg/kg	> 5620 5d+3d, Peking duck 2300 5d+3d, Coturnix virginianus (PESREG)
Effects on invertebrates	Filter paper test: LC50, 0.427 mg/cm2, 48hr, Eisenia foetida Artificial soil test: LC50, > 10000 mg/kg, 14d, Eisenia foetida OECD No 207 (PESREG)
Effects on microorganisms	Venzar (10-50 ppm, incubation 72hr) had no effect to the growth of Azotobacter chroococcum. (Pietr 1981)

EC50 values to algae, mg/l	0.012 0.014 0.015	72hr, EbC50, grw ihb 120hr, EbC50, grw ihb 24–48hr, ErC50, grw ihb Selenastrum capricornutum EPA, OECD No 201 (PESREG)
NOEC values to algae, mg/l	0.01	120hr, Selenastrum capricornutum EPA, OECD No 201 (PESREG)
EC50 values to crustaceans, mg/l	> 8.4 1.2 1.1 33	mg/l, 48hr, imb, Dapnia magna GLP, OECD No 202 (PESREG) 21d, imb, Daphnia magna 21d, rpd, Daphnia magna GLP, OECD No 202 (PESREG) 48hr, imb, Daphnia magna EPA, OECD No 202 (PESREG)
LOEC values to crustaceans, mg/l	0.97	21d, Daphnia magna GLP, OECD No 202 (PESREG)
NOEC values to crustaceans, mg/l	0.48 5.6	21d, Daphnia magna GLP, OECD No 202 (PESREG) 48hr, imb, Daphnia magna (PESREG)
LC50 values to fishes, mg/l	10 257 135 100< LC50< 1000	96hr, Cyprinus carpio (Pesticide Manual 1983) 48hr, Salmo gairdneri 96hr, Salmo gairdneri Lepomis macrochirus (PESREG)

1250 • Leptophos

21609-90-5

Synonyms	Leptofos O-(4-Bromo-2,5-dichlorophenyl)-O-methylphenylphosphonothioate	
Use	Insecticide.	
Log soil sorption coefficient, log Kom	3.97	(Sabljic 1987)
LC50 values to crustaceans, mg/l	22.6	96hr, Saccobranchus fossilis (Verma et al. 1982)

1251 • Limonene

138-86-3

Synonyms	1-Methyl-4-(1-methylethenyl) cyclohexane	
Sumformula of the chemical	C10H16	
EINECS-number	2053410	
Water solubility, mg/l	4	(MITI 1992)
Boiling point, °C	175.5–176.0	(MITI 1992)
Total degradation in water	Biodegradation: 41–98% by BOD (on the upward trend) period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

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1252 • Lindane

58-89-9

Synonyms	BHC HCCH HCH 1,2,3,4,5,6-Hexachlorocyclohexane γ-Hexachlorocyclohexane γ-BHC γ-HCH
Sumformula of the chemical	C6H6Cl6
Products containing the chemical	Benhexachlor Viton Gammexane Gexane Ben-Hex Aphtiria Aparasin Strevnex Tri-6 Laindatox Lorexane Kwell Quellada Jacutin
Use	Insecticide manufacturing, medicinal manufacturing (scabicide).
Odour	Odour threshold: detection: 12.0 mg/kg
Molecular weight	290.82
Specific gravity (water=1)	1.87 at 20/4 °C
Density, kg/m³	1850 20 °C
Water solubility, mg/l	17 24 °C 7.3–7.8 mg/l 20 °C (Anon. 1986b)
Melting point, °C	112
Boiling point, °C	323.4 (Anon. 1986b)
Log octanol/water coefficient, log Pow	3.85 (Anon. 1988) 3.72 (Anon. 1986b) 3.85 (Mackay 1982) 3.29 (Anon. 1989)
Henry's law constant, Pa x m³/mol	0.035 (Anon. 1988) 0.32 25 °C (Anon. 1989)
Adsorption/desorption	30–40% of lindane adsorbed on aquifer sand at 5 °C after 3 –100hr equilibrium time Desorption of lindane from aquifer sand: *mg lindane adsorbed /g of aquifer sand* — *% leached of total adsorbed lindane* 22.8 — 67.8 25.3 — 38.6 20.9 — 72.3 26.5 — 73.2 (Verschueren 1983)

Mobility	Equilibrium distribution: *mass %* air 0.58 water 47.66 solid 51.76 (Anon. 1988). Theoretical distribution: 47% water, > 50% sediment and soil (Nordic 1988).
Photochemical degradation in air	Stabile against photochemical degradation in atmosphere (IARC 1979).
Photochemical degradation in water	Photooxidation by ultra violet light in aqueous medium at 90–95 °C: - time for the formation of CO2 (% of theoretical): α γ 25% 4.2hr 3.0hr 50% 24.2hr 17.4hr 75% 40.0hr 45.8hr (Verschueren 1983). No photochemical degradation in river water in 8 weeks (Eichelberger & Lichtenberg 1971).
Half-life in soil, days	266 (Li et al. 1990)
Half-life in water, days	191 25 °C (Verschueren 1983)
Aerobic degradation in soil	Aerobic degradation in soil is very slow, 75–100% degradation: 3–10 years (Edwards 1966).
Total degradation in water	No degradation in bottle test, 28 days (Tabak al. 1981).
Degradation and transformation products	Dichlorobenzene trichlorobenzene tetrachlorobenzene pentachlorobenzene hexachlorobenzene (Anon. 1989).
Other information about degradation	Anaerobic dechlorination: 90% in 4 days (Haider & Jagnow 1975).
Metabolism in mammals	Effective uptake in alimentary canal and accumulation in fat tissue. Excretes mainly with urine in konjugated forms of di-, tri-, and tetrachlorophenols (IARC 1979).
Bioconcentration factor, fishes	167–727 (Verschueren 1983) 569 28d, Brachydanio rerio 35 35d, mussel, Lepomis macrochirus 477 304d, Pimephales promelas 70 261d, mussel, Salvelinus fontinalis 143 Rutilus rutilus, mussel, Inn 77 Rutilus rutilus, Donau 208 Rutilus rutilus, Main 500 Rutilus rutilus, Isar 2000 Angulilla anguilla, Isar 199 10d, Gasterosteus aculeatus (Anon. 1986b) 340–730 96hr, Cyprinodon (Schimmel et al. 1977) 470 304d, Pimephales (Macek et al. 1976) 600 Leuciscus (Rudolph & Boje 1988)
Bioconcentration factor, mollusca	100 Mytilus edulis (Verschueren 1983)

JKL

Bioconcentration factor, crustaceans	25–143 (Verschueren 1983) 34/46 24hr, Daphnia magna (Anon. 1986b) 38/72 72hr, Daphnia magna (Anon. 1986b) 30–140 96hr, Penaeus (Schimmel et al. 1977)
Bioconcentration factor, algae	433 Chlorella spec (Anon. 1986b) 671 Chlorella spec (Anon. 1986b)
Bioconcentration factor, other organisms	37000 sea water/Pacific white-sided dolphin (Lagenorhynchus obliquidens) (Virtanen & Nuuja 1987)
Other information about bioaccumulation	Confirmed to be accumulated on a medium level (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	76 orl-rat 25 orl-cat (Lewis & Sweet 1984) 88–91 orl-rat, acute (Verschueren 1983)
LD50 values to mammals in non-oral exposure, mg/kg	50 skn-rbt (Lewis & Sweet 1984) 900–1000 skn-rat, acute (Verschueren 1983)
TDLo values to mammals in oral exposure, mg/kg	111 orl (Lewis & Sweet 1984)
Effects on the reproduction of mammals	LOEL 0.5 mg/kg/day (4 months): impact on fertility and development of fetus (IARC 1979).
Other information about mammals	Approximated lethal dose to rat: 150 mg/kg (Virtanen & Nuuja 1987). When given in food to deer mouse (Peromyscus maniculatus) 1 mg/kg kills 50% in 4 days and 2 mg/kg kills 100% (Virtanen & Nuuja 1987).
Carcinogenicity	NCI carcinogenesis bioassay completed: results negative: mus, rat (Lewis & Sweet 1984). Highly carcinogenic to rats and mice (Verschueren 1983). Enough evidence of carcinogenicity to mice (IARC 1979).
Mutagenicity	Not mutagenic in tests with bacteria, yeast or Drosophila (IARC 1979).
LD50 values to birds in oral exposure, mg/kg	75 orl-Agelaius phoeniceus 100 orl-Sturnus vulgaris 56.2 orl-Passer domesticus ≥ 100 orl-Quiscalus quiscula 100 orl-Molothrus ater (Schafer et al. 1983)
LDLo values to birds in oral exposure, mg/kg	100 orl-bwd (Lewis & Sweet 1984)
Effects on invertebrates	Invertebrates: 0.026 mg/l, 10 d, change in species diversity (Lay et al. 1987).
Effects on bees	LD50, 0.0006 mg/bee (Torstensson 1988).
Effects on arthropods	LC50, Chironomus riparius: 0.330 mg/l, 2 d; 0.235 mg/l, 4 d (Green et al. 1986). LC50, 96hr, 0.004–0.175 mg/l (Anon. 1986b)
Effects on plants	EC50, Brassica rapa sativa rapifere, 66.5 mg/kg, 14d; EC50, Brassica rapa sativa rapifere, 760 mg/kg, 14d; EC50, Avena sativa, 426 mg/kg, 14d; EC50, Avena sativa, > 1000 mg/kg, 14d; (Anon. 1986b)

Effects on microorganisms	Pseudomonas putida: inhibition of cell multiplication starts at > 5 mg/l (Verschueren 1983). EC50, Photobacterium phosphoreum, 2.01 mg/l, 30 min (Anon. 1986b)
EC50 values to algae, mg/l	2.5 96hr, grw, Scenedesmus subspicatus (Geyer et al. 1985) 2.5 4d, Scenedesmus subspicatus 1.7/3.8 mg/l 4d, Scenedesmus subspicatus 0.2/0.3 mg/l, 4d, Chlorella spec (Anon. 1986b)
LOEC values to algae, mg/l	0.3 rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to crustaceans, mg/l	0.42 Daphnia pulex (Nishiuchi & Hashimoto 1967) 1.25 act, Daphnia pulex (Frear & Boyd 1967) 0.46 48hr, Daphnia magna (Sanders & Cope 1966, Frear & Boyd 1967) 0.72 48hr, Daphnia magna (Gorbach & Knauf 1971) 0.01 96hr, Gammarus fasciatus 0.01 96hr, Asellus brevicaudus (Sanders 1972) 0.00017 96hr, Penaeus duorarum (Schimmel et al. 1977) > 10 Daphnia pulex (Hashimoto & Nishiuchi 1981) 3.5 24hr, Daphnia magna (Bobacka et al. 1983) 0.46 Daphnia pulex (Pesticide manual 1983) 0.006-0.014 act, Gammarus pulex (Stephenson 1983) 1 48hr, Daphnia magna (Hermens et al. 1984) 0.005 96hr, Crangon septenspiosa (Eisler 1969) 0.54 96hr, Saccobranchus fossilis (Verma et al. 1982) > 0.430 2d, Asellus aquaticus 0.375 4d, Asellus aquaticus > 0.430 2d, Gammarus pulex 0.225 4d, Gammarus pulexcus (Green et al. 1986) 460–676 mg/l, 48hr, Cladocerena 0.010–0.048 mg/l, 96hr, Crustacea (Anon. 1986b)
EC50 values to crustaceans, mg/l	0.516 8hr, Daphnia magna 0.46 8hr, Daphnia pulex (Randall et al.1979) 0.34 16d, rpd, schr, Daphnia magna (Hermens et al.1984) 0.7 24hr, Daphnia magna (Anon. 1986b)
NOEC values to crustaceans, mg/l	15 chr, Daphnia (Macek et al. 1976a) 0.1 21d, rpd, Daphnia magna 0.055 21d, rpd, Daphnia magna 0.439–0.625 mg/l, 21d, rpd, Daphnia magna 0.1550–0.218 mg/l, 21d, rpd, Daphnia magna (Anon. 1986b)

JKL

LC50 values to fishes, mg/l	0.17	48hr, Cyprinus carpio (Nishiuchi & Hashimoto 1967)
	0.009	96hr, Menidia menidia (Eisler 1970a)
	0.027	96hr, Salmo gairdneri
	0.002	96hr, Salmo trutta m.lacustris
	0.041	96hr, Perca fluviatilis (Macek & McAllister 1970)
	0.057	96hr, Lepomis macrochirus (Randall et al.1979)
	0.31	48hr, Cyprinus carpio
	0.12	48hr, Carassius auratus (Hashimoto & Nishiuchi 1981)
	0.14	96hr, Trichogaster trichopterus (Ramalingam & Reddy 1982)
	3.2	48hr, Tilapia sp. (Basha et al. 1983)
	0.075	96hr, Gobio gobio (Marcelle & Thome 1983)
	0.068	act, Lepomis macrochirus
	0.27	act, Salmo gairdneri
	0.087	act, Pimephales promelas (Pesticide Manual 1983)
	0.016	96hr, Poecilia reticulata (Gupta et al. 1984)
	0.340–0.670	1d, Anguilla anguilla
	0.320–0.670	4d, Anguilla anguilla (Ferrando et al. 1987)
	16	4d, Clarias batrachus (Singh & Singh 1987a)
	0.28/0.03	mg/l, 48hr, Leuciscus idus melanotus (Anon. 1986b)
	0.06/0.09	mg/l, 48hr, Brachydanio rerio (Anon. 1986b)
	0.022	96hr, Salmo gairdneri (Tooby & Hursey 1975)
LOEC values to fishes, mg/l	0.024	srv, chr, Pimephales promelas (Macek et al. 1976a)
	0.017	grw, rpd, schr, Salvelinus fontinalis (Macek et al. 1976c)
	0.0008	28d, fish (Rudolp & Boje 1988)
NOEC values to fishes, mg/l	0.009	srv, chr, Pimephales promelas (Macek et al. 1976a)
	0.009	srv, schr, Salvelinus fontinalis (Macek et al. 1976c)
	16.5	chr, Pimephales promelas (Macek et al. 1976b)
	0.0008	28d, Brachydanio rerio
	0.008	14d, Brachydanio rerio
	0.011	14d, Brachydanio rerio
	0.02	14d, Brachydanio rerio
	0.03	14d, Brachydanio rerio
	0.002–0.142	96hr (Anon. 1986b)
Effects on the physiology of water organisms	Anabas testudineus; 0.075 mg/l, histological effect (presence of physical damage to tissues) (Bakthavathsalam et al. 1987). Biochemical effect (change in physiochemical process including glycogen uptake, cholesterol levels and lipid analysis): Clarias batrachus, 0.002 mg/l, 28 d (Lal & Singh 1987); Cyprinus carpio, 0.1 mg/100g/d, 10 d (Kobayashi et al. 1987). Heteropneustes fossilis, 8 mg/l, 4 d, change in enzyme activity, change in hormone concentration (Yadav & Singh 1987).	

Other information about water organisms	Microcystis aeruginosa: inhibition of cell multiplication starts at 0.3 mg/l (Verschueren 1983). LC50 48hr: 7.3 ppm Lymnea stagnalis, at 2 ppm: decrease in growth rate from third month; 60% decrease of fecundity Lymnea stagnalis L.: rearing of larvae is impossible at 2 mg/l Pteronarcys californica: 96hr LC50 4.5 µg/l fourth instar larval Chironomus riparius: 24hr LC50 3.6 µg/l insect larvae (Chaoborus): 48hr LC50 0.008 ppm (Cloeon): 0.092 ppm (Verschueren 1983) LC50 (24hr), 0.0036 mg/l, Chironomus riparius (Sanders & Cope 1968). LOEC, 10 mg/l, srv, act, Colpidium campylum (Dive et al. 1980). LC50, Physa fontinalis: > 0.430 mg/l, 2 d, 4 d (Green et al. 1986). Algae: 0.435 mg/l, 10 d, change in biomass (Lay et al. 1987).

1253 • Linear alkylbenzene 123-01-3

Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

1254 • Linear alkylbenzene sulfonate 42615-29-2

Synonyms	LAS	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
EC50 values to algae, mg/l	50–100	48hr, rpd, Selenastrum capricornutum (Atsuko et al. 1984)
LC50 values to crustaceans, mg/l	4.8	48hr, Daphnia magna (Lewis 1983)
EC50 values to crustaceans, mg/l	2.2–10.1	48hr, Daphnia magna (Barera & Adams 1983)
LC50 values to fishes, mg/l	5	96hr, Salmo gairdneri (Pohla-Gubo & Adam 1982) * C 10–15, activity 46.7%
	0.7	96hr, Rasbora heteromorpha
	0.1–0.5	96hr, Salmo trutta
	0.4–0.6	96hr, Leuciscus idus
	1.2	48hr, Carassius auratus (Reiff et al. 1979)
LOEC values to fishes, mg/l	1.2	srv, chr, Pimephales promelas (Pickering & Thatcher 1970)
	8.4	C 11.2, srv, chr, Pimephales promelas
	4.8	C 11.7, srv, schr, Pimephales promelas
	2.5	C 13.3, srv, chr, Pimephales promelas (Holman & Macek 1980)
NOEC values to fishes, mg/l	6.3	srv, chr, Pimephales promelas (Pickering & Thatcher 1970)
	5.1	C 11.2, srv, chr, Pimephales promelas
	3.1	C 11.7, srv, schr, Pimephales promelas (Holman & Macek 1980)
Effects on the physiology of water organisms	Cirrhinus mrigala, 0.005 mg/l, 30 d, histological effect (presence of physical damage to tissues) (Misra et al. 1987).	
Other information about water organisms	Oryzias latipes, 0.013 mg/l , 0.03 d, avoidance or attraction to a chemical gradient (Hidaka & Tatsukawa 1986).	

1255 • Linevol

83968-18-7 (Linevol 79)

Synonyms	Phthalic acid, dialkyl (C7–9) ester (Linevol 79)	
LC50 values to fishes, mg/l	9	24hr, Linevol 79, Carassius auratus
	3	24hr, Linevol 911, Carassius auratus (Verschueren 1983)

1256 • Linuron

330-55-2

Synonyms	3-(3,4-Dichlorophenyl)-1-methoxy-1-methylurea N-(3,4-Dichlorophenyl)-N'-methoxy-N'-methylurea	
Use	Active ingredient in herbicides.	
Water solubility, mg/l	75	(MITI 1992)
Melting point, °C	93–94	(MITI 1992)
Log octanol/water coefficient, log Pow	3.07	(MITI 1992)
Half-life in soil, days	75	(Li et al. 1990)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	15–20	6w, Cyprinus carpio, conc 0.2 mg/l
	13–23	6w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
Effects on plants	1.0 kg linuron /ha was applied with a sprayer following seeding (preemergence) to lamb's-quarters (Chenopodium album L.) →plants (seeds) were killed (Jensen et al. 1977)	
	Linuron was sprayed to soil shortly after sowing →50% inhibition of CO2 fixation was attained in one-week-old plants (maize, Zea mays) with a dose corresponding to 0.85 kg/ha linuron. (Muschinek et al. 1979).	
	Postemergence application of 50 g linuron /are (5kg/ha) within 30 days decreased both survival and the fresh weight of onions (Giannopolitis 1982).	
LC50 values to crustaceans, mg/l	13.7	48hr, Daphnia magna (Bogacka et al. 1983)
LC50 values to fishes, mg/l	16	96hr, Salmo gairdneri Lepomis macrochirus (Pesticide Manual 1983)
	33.1	24hr, Lebistes reticulatus (Bogacka et al. 1983)
	32	48hr, Oryzias latipes (MITI 1992)

1257 • Lithium and lithium compounds

7439-93-2

LC50 values to fishes, mg/l	9.28	28d, Salmo gairdneri (Birge et al. 1980)

JKL

1258 • Magnesium and magnesium compounds 7439-95-4

LC50 values to crustaceans, mg/l	190 140 322 720	21d, Daphnia magna 48hr, without food, D.magna 48hr, with food, D.magna (Biesinger & Christensen 1972) 96hr, Nitocra spinipes (Bengtsson 1978)
EC50 values to crustaceans, mg/l	125	21d, rpd, Daphnia magna (Biesinger & Christensen 1972)
LOEC values to crustaceans, mg/l	82	21d, rpd, Daphnia magna (Biesinger & Christensen 1972)
LC50 values to fishes, mg/l	1355	28d, Salmo gairdneri (Birge et al. 1980)

1259 • Malachite green 569-64-2

Synonyms	Basic Green-4	
Molecular weight	364.95	
Water solubility, mg/l	> 1000	(MITI 1992)
Log octanol/water coefficient, log Pow	-0.17	(MITI 1992)
Total degradation in water	Biodegradation: 0.3% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	36–91 44–75	8w, Cyprinus carpio, conc 0.02 mg/l 8w, Cyprinus carpio, conc 0.002 mg/l (MITI 1992)
LD50 values to mammals in oral exposure, mg/kg	80	orl-mus (Lewis & Sweet 1984)
LC50 values to fishes, mg/l	0.25 0.03 0.22 0.045 0.3 0.27 2.86 0.32	96hr, Salmo gairdneri 96hr, Lepomis macrochirus 96hr, Salmo trutta m. lacustris 96hr, Micropterus dolomieu (Bills et al. 1977) 48hr, Oryzias latipes (Tonogai et al. 1982) 96hr, Anguilla rostrata 96hr, Anguilla rostrata (Hinton & Eversole 1978) 48hr, Oryzias latipes (MITI 1992)

1260 • Malaoxon 1634-78-2

Synonyms	S-(1,2-Diethoxycarconyl)ethyl-0,0-dimethylphosphorothioate
Other information about water organisms	LC50 (24hr), 0.0054 mg/l, Chironomus riparius (Estenik & Collins 1979).

MNO

1261 • Malathion

121-75-5

Synonyms	S-(1,2-Di(ethoxycarbonyl)-ethyl)-O,O-dimethylphosphorodithioate
Use	Active ingredient in insecticides, acaricide.
Molecular weight	330.38
Vapour pressure, mmHg	0.00004 20 °C
Water solubility, mg/l	145 20 °C
Melting point, °C	2.85
Boiling point, °C	156–157
Log octanol/water coefficient, log Pow	2.9 (Anon. 1988)
Henry's law constant, Pa x m³/mol	0.012 (Anon. 1988)
Mobility	Equilibrium distribution: *mass %* air 0.36 water 88.82 solid 10.82 (Anon. 1988).
Hydrolysis in water	No hydrolysis found after 12 days (pH 5–7) (Verschueren 1983).
Half-life in soil, days	1 (Li et al. 1990)
Total degradation in water	0% of original compound found after 4 weeks in river water (initial concentration 0.010 mg/l) (Verschueren 1983).
LD50 values to mammals in oral exposure, mg/kg	250 orl-rbt 53 orl-ctl (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	4100 skn-rbt (Lewis & Sweet 1984)
LDLo values to mammals in oral exposure, mg/kg	246 orl-wmn (Lewis & Sweet 1984)
Carcinogenicity	NCI carcinogenesis bioassay completed: results negative; mus, rat (Lewis & Sweet 1984).
LD50 values to birds in oral exposure, mg/kg	600 orl-ckn 1.485 orl-dck (Lewis & Sweet 1984) 400 orl-Agelaius phoeniceus (Schafer et al. 1983)
Effects on amphibia	LC50 (96hr), 0.0006 mg/l, tadpoles of Rana hexadactyla (Khangarot et al. 1985).

LC50 values to crustaceans, mg/l	0.5	48hr, Penaeus duorarum (Butler 1963)
	0.033	48hr, Daphnia magna (Hermens et al. 1984)
	0.00076	96hr, Gammarus fasciatus
	0.001	96hr, Gammarus lacustris (Sanders 1972)
	0.000023	30d, Gammarus pseudolimneaus (Verschueren 1983)
	0.08	96hr, Palaemon macrodactylus (Earnest 1971)
	0.03	96hr, Crangon septemspinosa (Eisler 1969)
	0.33–1	Crangon crangon (Connor & Portmann 1965)
	1.63	48hr, Macrobrachium lamarrei (Nagabhushanam et al. 1983)
	9.79	96hr, Saccobranchus fossilis (Verma et al.1982)
	0.0009	act, Daphnia pulex (Frear & Boyd 1967)
	0.003	48hr, Daphnia magna (Gorbach & Knauf 1971)
	0.013	act, Daphnia pulex (Nishiuchi & Hashimoto 1967)
	0.012	24hr, Daphnia magna
	0.009	48hr, Daphnia magna (Ardo 1974)
	0.0009	act, Daphnia magna (Kenaga 1979)
EC50 values to crustaceans, mg/l	0.0008–0.0018	48hr, Daphnia pulex (Frear & Boyd 1967)
	0.00036	rpd, 16d, Daphnia magna (Hermens et al. 1984)
LC50 values to fishes, mg/l	0.1	96hr, Oncorhynchus kisutch
	0.26	96hr, Perca fluviatilis
	0.17	96hr, Salmo gairdneri (Macek & McAllister 1970)
	0.001	96hr, Acroneuria lycorias (Sanders 1972)
	0.027	96hr, Thalassoma bifasciatum
	0.08	96hr, Fundulus heteroclitus (Eisler 1970a)
	0.367	48hr, Sarotheredon (Basha et al. 1983)
	2.5	96hr, Cyprinus carpio (Singh et al. 1981)
	4.5	48hr, Cyprinus carpio (Nishiuchi & Hashimoto 1967)
	0.103	act, Lepomis macrochirus
	0.17	act, Salmo gairdneri
	8.65	act, Pimephales promelas (Kenaga 1979)
	12	4d, Clarias batrachus (Singh & Singh 1987a)
	0.16	4d, Salmo gairdneri (McKim et al. 1987)
LOEC values to fishes, mg/l	0.007	srv, chr, Lepomis macrochirus (Eaton 1970)
	0.037	srv, chr, Lepomis macrochirus (Ward & Parrish 1980)
	0.009	srv, schr, Lepomis macrochirus (Parrish et al. 1977)
	0.58	srv, chr, Pimephales promelas (Mount & Stephan 1967)
	0.011	srv, grw, chr, flagfish (Hermanutz 1978)
NOEC values to fishes, mg/l	0.004	srv, chr, Lepomis macrochirus (Eaton 1970)
	0.004	srv, schr, Lepomis macrochirus (Parrish et al. 1977)
	0.2	srv, chr, Pimephales promelas (Mount & Stephan 1967)
	0.009	srv, grw, chr, flagfish (Hermanutz 1978)

MNO

Effects on the physiology of water organisms	Clarias batrachus, 28 d: 0.001 ml/l, biochemical effect (change in physiochemical process including glycogen uptake, cholesterol levels and lipid analysis) (Lal & Singh 1987); 1.0 mg/l, change in hormone concentration (Singh & Singh 1987a, 1987b). Heteropneustes fossilis; 10.0 mg/l, 4 d, change in enzyme activity, change in hormone concentration (Yadav & Singh 1987). Lamellidans corrianus, 0.020–0.120 mg/l, 4 d, change in oxygen uptake of test animal or tissue (Muley & Mane 1987). Oziotelphusa senex senex, 2 mg/l, 10 d, change in physiochemical process including glycogen uptake, cholesterol levels and lipid analysis (Reddy et al. 1986).
Other information about water organisms	LC50 (48hr), 13.4 mg/l, Mytilus edulis, embryo (Liu & Lee 1975). Salmo gairdneri, 0.296 mg/l, 1.67 d, lethal threshold concentration (LT50) (McKim et al. 1987).

1262 • Maleic acid

110-16-7

Sumformula of the chemical	C4H4O4	
Molecular weight	116.07	
Water solubility, mg/l	788000	25 °C (Suntio et al. 1988)
Melting point, °C	138–139 (Weast 1982–83)	
pKa	0.076	(Weast 1982–83)
Log octanol/water coefficient, log Pow	-0.79	(Verschueren 1983)
LD50 values to birds in oral exposure, mg/kg	> 98	orl-Agelaius phoeniceus (Schafer et al. 1983)
LC50 values to fishes, mg/l	5	96hr, Pimephales promelas (Kemp et al. 1973)

MNO

1263 • Maleic anhydride

108-31-6

Synonyms	cis-Butenedioic anhydride Dihydro-2,5-dioxofuran Maleic acid anhydride	
Sumformula of the chemical	C4H2O3	
Molecular weight	98.06	
Vapour pressure, mmHg	0.41	at 25 °C (Daubert & Danner 1985)
Melting point, °C	52.7-52.8 (MITI 1992)	
Boiling point, °C	202 202.2	(Howard I 1990) (MITI 1992)
Volatilization	Maleic anhydride should not volatilize appreciable from water or moist soil due to its rapid hydrolysis. Volatilization from dry soil or surfaces should be slow due to its relatively low vapour pressure (Howard 1989). Decomposes (Weast 1986).	
Photochemical degradation in air	Although maleic anhydride absorbs UV radiation above 290 nm, no information could be found concerning its photolysis (Howard 1989). Maleic anhydride readily reacts with ozone and hydroxyl radicals in the atmosphere, estimated atmospheric half-life is 1.7hr (Cupitt 1980).	

Other reactions in atmosphere	In the vapour phase hydrolysis is completed in 21hr at 96% relative humadity, while no hydrolysis occurs at 50% relative humidity (Rosenfeld & Murphy 1967). Maleic anhydride readly reacts with ozone and hydroxyl radicals in the atmosphere, estimated atmospheric half-life is 1.7hr (Cupitt 1980).
Hydrolysis in water	Maleic anhydride hydolyzes rapidly in water at room temperature to give maleic acid (half-life 0.37 min, at 25 °C in initially neutral solution) (Bunton et al. 1963).
Total degradation in water	Biodegradation: 55% by BOD (on the upward trend) period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
Other information about degradation	It was obtained 68.9 and 74.0% theoretical BOD in fresh and salt water, respectively (Takemoto et al. 1981). It was reported that 99% removal was achieved in 4hr by activated sludge (Matsui 1975). It was reported that 40–60% theoretical BOD in 5 days with sewage inoculum (Heukelekian & Rand 1955) (Verschueren 1983). Maleic anhydride has been characterized as biodegradable during biological sewage treatment (Thom & Agg 1975).
LC50 values to fishes, mg/l	235 96hr, Gambusia affinis (Jones 1971) 150 24hr, Lepomis macrochirus (Turnbull et al. 1954)

1264 • Maleic hydrazine 123-33-1

Use	Plant growth regulator.
LC50 values to crustaceans, mg/l	107 96hr, Daphnia spp. (Pesticide Manual 1983)
LC50 values to fishes, mg/l	100 96hr, Rasbora heteromorpha (Tooby et al. 1975) 1608 Lepomis macrochirus 1435 96hr, Salmo gairdneri (Pesticide Manual 1983)

1265 • Malononitrile 109-77-3

Synonyms	Dicyanomethane
LC50 values to fishes, mg/l	1.6 96hr, Salmo gairdneri (Abram & Wilson 1979)

1266 • Mancozeb 8018-01-7

Synonyms	Mancofol Manzeb Dithane M-45 * Carbamic acid, ethylenebis(dithio-, manganese zinc complex)
Sumformula of the chemical	C4H6MnN2S4.C4H6N2S4Zn
Products containing the chemical	Dithane M-45 * mancozeb 800g/kg (PESREG)
Chemicals in the product	manganese * 16%; zinc * 2%; ethylenebisdithiocarbamate ion * 62 %; or; manganeseethylenebisdithiocarbamate; and; zinc ion

Use	Active ingredient in fungicides.
Molecular weight	541.03
Vapour pressure, mmHg	0.001333 < 0.01 mPa (KEMI 1990)
Water solubility, mg/l	16 at 25 °C (KEMI 1990)
Log octanol/water coefficient, log Pow	1.34 (KEMI 1990)
Mobility	The leaching behaviour of Dithane M-45 (10 lb/a) was studied (one inch of water per week for nine weeks) in the soil (five different soils) columns. Most of Dithane M-45 retained in the upper one inch, but it was found 1.8–4.3% of applied radioactivity from the leachate water of clay soil. In the study part of Dithane M-45 did lost from the soils by volatilization. (PESREG) In the soil column studies it was discovered low mobility for mancozeb in silt and clay soils. In soils with low organic material there is expected mobility for mancozeb and degradation product ETU (ethylenethiourea) from medium to very high. Koc: 363–2334 for mancozeb and Koc: 34–146 for ETU. (KEMI 1990) Decomposition at 192–204 °C. (KEMI 1990)
Photochemical degradation in soil	Mancozeb is photolysis stabile. (KEMI 199)
Hydrolysis in water	The half-life of Dithane M-45 was about 17 hours (pH 7, 25 °C) and the hydrolyse products were ethylenebisisothiocyanate sulfide (EBIS) ethylenethiourea (ETU) and ethyleneurea (EU). (PESREG)
Hydrolysis in acid	The half-life of Dithane M-45 was about 20 hours (pH 5, 25 °C) and the major hydrolyse products were ethylenethiourea (ETU) and ethyleneurea (EU). (PESREG)
Hydrolysis in base	The half-life of Dithane M-45 was about 34 hours (pH 9, 25 °C) and the major hydrolyse products were ethylenethiuram disulfide (ETD), ethylenethiourea (ETU) and ethyleneurea (EU). (PESREG)
Aerobic degradation in soil	In the degradation of (C-14) mancozeb (10 ppm and 20 ppm) was studied in the silt loam soil under nonsterile and sterile aerobic conditions. The half-life of mancozeb was less than two days. The degradation of mancozeb went via the intermediates etylenebisisothiocyanate sulfide (EBIS) and ethylenethiourea (ETU) to ethyleneurea (EU). The half-life of ETU was also less than two days, degrading rapidly to EU. Mancozeb degradates are mineralized to 14CO2 in non-sterile aerobic soil. Mineralization half-lifes of mancozeb (20 ppm and 10 ppm) were 90–105 days. Anaerobic conditions were established after 30 days of aerobic conditions. EU was the primary soil metabolite at the start of the anaerobic study. 2-imidazoline was found found as a degradation product in anaerobic study. (PESREG) Under aerobic conditions and in moist soils there is rapid chemical and biological degradation (< 2 days) of mancozeb and ETU to ethyleneurea. Mineralization half-life has been estimated to about 100 days. (KEMI 1990)
Anaerobic degradation in soil	See aerobic degradation in soil.
Total degradation in water	In water is happening a relative quick chemical degradation nearest through oxidation. (KEMI 1990)
Degradation and transformation products	ethylenethiuram disulfide (ETD) ethylenebisisothiocyanate (EBIS) ethylenethiourea (ETU) ethyleneurea (EU) 2-imidazoline
LD50 values to mammals in oral exposure, mg/kg	7500 orl-rat (Lewis & Sweet 1984) 5000–14000 orl-rat (KEMI 1990)

MNO

LD50 values to mammals in non-oral exposure, mg/kg	600	unk-mus (Lewis & Sweet 1984)
	> 5000	idr-rbt, idr-rat (KEMI 1990)
LC50 values to mammals in inhalation exposure, mg/m³	> 5.14	mg/l, ihl-rat (KEMI 1990)
TDLo values to mammals in oral exposure, mg/kg	1320	orl-rat, 11d, preg. (Lewis & Sweet 1984)
Other information about mammals	NOEL, 14d, 11 µg/l, rat. (KEMI 1990)	
LD50 values to birds in oral exposure, mg/kg	> 6400	Anas platyrhynchos (KEMI 1990)
Effects on reptiles	LC50, 14d, > 300 mg/kg, earthworm. (KEMI 1990)	
Effects on invertebrates	LC50, 7d, 14d, Eisenia foetida, GLP, OECD No 207: The results indicate that Dithane M-45 is of low toxicity to earthworms at concentrations of 3.0–299.1 ppm a.i. in soil (1.9–190.0 kg a.i./ha) (PESREG)	
Effects on bees	LD50, > 193 µg/bee. (KEMI 1990)	
EC50 values to microorganism, mg/l	0.08	15 min Microtox (Van Leeuwen et al. 1985)
	32	Nitrification (Van Leeuwen et al. 1985)
EC50 values to algae, mg/l	2.8	96hr, inb grw, Scenedesmus subspicatus Chodat, 80% mancozeb (PESREG)
EC50 values to crustaceans, mg/l	13.6	24hr, mbt, Daphnia magna, Dithane M-45 * (PESREG)
	0.9	24hr, mbt, Daphnia magna (KEMI 1990)
NOEC values to crustaceans, mg/l	0.006	21d, rpd, Daphnia magna (KEMI 1990)
LC50 values to fishes, mg/l	24	48hr, Cyprinus carpio
	1.9	48hr, Salmo gairdneri (Hejduk & Svobodova 1980)
	7.7	48hr, Carassius auratus
	4.5	48hr, Ictalurus nebulosus
	24	48hr, Cyprinus carpio
	2.2	48hr, Poecilia reticulata (Pesticide Manual 1983)
	1.9	48hr, Salmo gairdneri (PESREG)
	7.7	48hr, Carassius auratus (PESREG)
	4.5	48hr, Ictalurus nebulosus (PESREG)
	2.31	96hr, Phoxinus phoxinus L (PESREG)
	1.5–2.3	mg/l, 96hr (KEMI 1990)
NOEC values to fishes, mg/l	0.005	33d, grw, Rhombus maximus (KEMI 1990)
Other information about water organisms	0.01< TL50< 0.10 mg/l, 48 hour, Crassostrea virginica (the concentration of Dithane M-45 which inhibited normal development of 50% of the developeng oyster larvae). No effect on normal embryonic development was observed among oyster larvae (Crassostrea virginica) exposed to Dithane M-45 at 0.01 mg/l for 48 hours. (PESREG) The acute toxicity of Dithane M-45	

	TL50 (mg/l) 96hr	*No effect level (mg/l)*
Palaemonetes vulgaris	> 10.0, < 18.0	10.0
Uca pugilator	> 1000	1000
(PESREG)		

EC50, 48hr, 0.48 mg/l, oyster. (KEMI 1990)

1267 • Maneb 12427-38-2

Synonyms	Manganeseethylene-1,2-bis-dithiocarbamate Maneba * Ethylenebis(dithiocarbamic acid) manganous salt Manganousethylenebis(dithiocarbamate)
Sumformula of the chemical	C4H6MnN2S4
Products containing the chemical	Maneba * maneb 800 g/kg (PESREG)
Use	Active ingredient in fungicides.
Way to effect	Contact function (PESREG).
Instruction for handling	Stable at least 2 years in unopened, undamaged original package (PESREG).
State and appearance	Yellow, odourless solid. Wettable powder (Manabe *) (PESREG)
Particle size, mm	0.045 refuse to the sieve: 2.93% (PESREG)
Molecular weight	266.31
Density, kg/m³	400–500, 0.4–0.5 g/cm³ (PESREG)
Degradation point, °C	approx. 135 °C (PESREG)
Other physicochemical properties	Insoluble in water, fat and most organic solvents. (PESREG)
Aerobic degradation in soil	The degradation of maneb was studied under aerobic conditions in two soils (sandy loam, loamy sand). After 32 days and 30 days, respectively, of aerobic incubation 15.9% (loamy sand) and 22.82% (sandy loam) of the applied radioactivity were mineralized and analyzed as 14C02. The degradation products ethylenethiourea, ethyleneurea, ethylenebis (isothiocyanate) sulfide and carbimid were identified in the soils. (PESREG)
Anaerobic degradation in water	Under laboratory conditions maneb (10 ppm, 25 °C) rapidly degraded in an anaerobic aquatic system (water and sediment). Degradation was so rapid that a half-life for maneb could not be determined. Three major identified products were ethylenebis (isothiocyanate) sulfide, ethylenethiourea and ethyleneurea. The estimated half-life for degradation of ethylenethiourea in an anaerobic aquatic system was 149 days. (PESREC)
Degradation and transformation products	1, H-imidazole-2-thione, 4,5-dihydro = (ethylenethiourea); 2-imidazolidinone = (ethyleneurea); 3, H-imidazole-(2,1-c)-1,2,4-dithiazole-3-thione, 5,6-dihydro = ethylenebis (isothiocyanate) sulfide; 1, H-imidazole-2-thione, 4,5-dihydro, 1-thioformamido = carbimid (PESREG)
LD50 values to mammals in oral exposure, mg/kg	4500 orl-rat 4000 orl-mus (Lewis & Sweet 1984) 8760 orl-rat (PESREG) 4900 orl-rat, Maneba * (PESREG)
LD50 values to mammals in non-oral exposure, mg/kg	> 5000 mg/kg, idr-rat (PESREG) > 5000 mg/kg, idr-rat, Maneba * (PESREG) 190 ipr-rat (PESREG)
LD50 values to birds in oral exposure, mg/kg	> 100 orl-Agelaius phoeniceus (Schafer et al. 1983) 1467 orl-bdw, 14d, Colinus virginianus > 4640 14d, orl-bdw, Anas platyrhynchos (PESREG)

MNO

Effects on invertebrates	LC50, 840 ppm, 14d, Eisenia foetida (PESREG) NOEC, 200 ppm, 14d, Eisenia foetida (PESREG)	
Effects on plants	11.2 kg maneb (80%)/ha when sprayed to soil depressed growth of mycorrhizal sour orange (Citrus aurantium) seedlings (Nemec 1980).	
EC50 values to microorganism, mg/l	1.2 56	15 min Microtox (Van Leeuwen et al. 1985) Nitrification (Van Leeuwen et al. 1985)
EC50 values to algae, mg/l	3.2	rpd, 96hr, Chlorella pyrenoidosa (Leeuwen et al. 1985)
	0.3	grw, 96hr, Chlorella fusca (PESREG)
NOEC values to algae, mg/l	0.06	Chlorella fusca (PESREG)
LC50 values to crustaceans, mg/l	1	48hr, Daphnia magna (Leeuwen et al. 1985)
	3.3	48hr, Crangon crangon (Kemp et al. 1973)
	0.11	21d, Daphnia magna (van Leeuwen et al. 1987)
	1.02	48hr, Daphnia magna (PESREG)
EC50 values to crustaceans, mg/l	0.06	Daphnia magna (van Leeuwen et al. 1987)
LC50 values to fishes, mg/l	0.53	96hr, Rasbora heteromorpha (Tooby et al. 1975)
	1.8	48hr, Cyprinus carpio (Pesticide Manual 1983)
	3.7	96hr, Poecilia reticulata (Leeuwen et al. 1985)
	3.05 0.22	96hr, Cyprinum carpio (PESREG) 96hr, Salmo gairdneri (PESREG)

1268 • Manganese and manganese compounds 7439-96-5

Effects on plants	200 ppm Mn in barley leaves →tissue injury (Gupta et al. 1973).	
EC50 values to algae, mg/l	3.1	rpd, schr, Selenastrum capricornutum (Christensen et al. 1979)
LC50 values to crustaceans, mg/l	333 771	Mn(II), 96hr, mbt, Asellus aquaticus Mn(II), 48hr, mbt, Asellus aquaticus (Martin & Holdich 1986)
	5.7 9.8	21d, Daphnia magna 48hr, without food, D.magna (Biesinger & Christensen 1972)
EC50 values to crustaceans, mg/l	5.2	21d, rpd, Daphnia magna (Biesinger & Christensen 1972)
LOEC values to crustaceans, mg/l	4.1	21d, rpd, Daphnia magna (Biesinger & Christensen 1972)
LC50 values to fishes, mg/l	2.91	28d, Salmo gairdneri (Birge et al. 1980)

1269 • Manganese carbonate 598-62-9

Effects on the physiology of water organisms	Cyprinus carpio, 0.0131 mg/g, 140 d, measurable change in length and/or weight (Satoh et al. 1987a).

1270 • Manganese chloride 7773-01-5

EC50 values to crustaceans, mg/l	771 333 1389 694	mbt, 2d, Asellus aquaticus mbt, 4d, Asellus aquaticus mbt, 2d, Crangonyx pseudogracilis mbt, 4d, Crangonyx pseudogracilis (Martin & Holdich 1986)
Effects on the physiology of water organisms	Cyprinus carpio, 0.013 mg/g, 140 d, measurable change in length and/or weight (Satoh et al. 1987a).	

1271 • Manganese(II) sulfate 7785-87-7

Synonyms	Manganese sulfate Manganese(2+) sulfate Sulfuric acid, manganese(II) salt	
Sumformula of the chemical	O4S.Mn	
Molecular weight	151	
LDLo values to mammals in oral exposure, mg/kg	332	ipr-mus (Sweet 1987)
TDLo values to mammals in non-oral exposure, mg/kg	50 25 660	ipr-mus, 10d preg. effects on embryo or fetus ipr-mus, 8d preg. specific developmental abnormalities ipr-mus, tumorigenic (Sweet 1987)
Mutagenicity	Mutation data: DNA inhibition, smc, 10 mmol/l; dnr, bsc, 50 mmol/l; microbial mutation without S9, microorganisms, 10 mmol/l; sin, smc, 3 mmol/l (Sweet 1987).	
Effects on the physiology of water organisms	Cyprinus carpio, 0.0128 mg/g, 140 d, measurable change in length and/or weight (Satoh et al. 1987a).	

MNO

1272 • Manganese oxide 1313-13-9

Effects on the physiology of water organisms	Cyprinus carpio, 0.0137 mg/g, 140 d, measurable change in length and/or weight (Satoh et al. 1987a).

1273 • D-Mannitol 69-65-8

Synonyms	1,2,3,4,5,6-Hexanehexol Manna sugar Mannite Osmitrol	
Sumformula of the chemical	C6H14O6	
LD50 values to mammals in oral exposure, mg/kg	22000 13500	orl-mus orl-rat (Sweet 1987)

LD50 values to mammals in non-oral exposure, mg/kg	14000 7470 9690	ipr-mus ivn-mus ivn-mus (Sweet 1987)
TDLo values to mammals in non-oral exposure, mg/kg	17143	ivn-man, vascular, gastrointestinal, kidney, ureter, bladder (Sweet 1987)
Carcinogenicity	NTP carcinogenesis bioassay (feed); no evidence: mouse, rat (Sweet 1987).	
Mutagenicity	Mutation data: DNA inhibition, human, lymphocyte, 50 mmol/l (Sweet 1987).	

1274 • MCPA

94-74-6

Synonyms	2-Methyl-4-chlorophenoxyacetic acid	
Use	Active ingredient in herbicides.	
Way to effect	Hormonic type (Hattula 1979).	
Molecular weight	200.63	
Water solubility, mg/l	730	acid
Total degradation in soil	75–100% disappearance from soils during 3 months (Verschueren 1983).	
LD50 values to mammals in oral exposure, mg/kg	700 550	orl-rat orl-mus (Lewis & Sweet 1984)
Effects on plants	Aspen plants (Populus tremula) were grown in 0.000001 M MCPA solution → swelling of the stem base, time of survival > 25 days. (0.00001 M → epinastic curvatures, necrosis of the leaves, swelling of the stem base, time of survival 16 days) (Eliasson 1963). Postemergence application of 16.8 kg MCPA/are (= 1.680 kg/ha) within 30 days caused severe swelling and twisting of onion roots (Giannopolitis 1982). Seeds of pure wheat (Tritium sativum), rye (Secale cereale) and maize (Zea mays) were grown 6 weeks in soil containing 10 ppm MCPA → a significant decrease in germination percentage, increasing amounts of abnormalities at the root systems (Sattar & Paasivirta 1979).	
LC50 values to crustaceans, mg/l	11	96hr, Daphnia magna (Knapek & Lakola 1974)
	16	48hr, Crassostrea virginica (Davis & Hidu 1969)
	> 40	act, Daphnia pulex (Nishiuchi & Hashimoto 1967)
LC50 values to fishes, mg/l	1.5	48hr, Lepomis macrochirus (Hughes & Davis 1964)
	25 59	96hr, Salmo trutta m. fario 96hr, Cyprinus carpio (Knapek & Lakola 1974)
	100	48hr, Lepomis macrochirus (Edwards 1977)
	460	24hr, Carassius auratus (Bridie et al. 1979)
	944	48hr, Lebistes reticulatus (Bogacka et al. 1983)
	> 40	48hr, Cyprinus carpio (Nishiuchi & Hashimoto 1967)
Other information about water organisms	LC50 (96hr), 335 mg/l, Mosquito (larvae) (Knapek & Lakola 1974).	

1275 • MCPB

94-81-5

Synonyms	4-(4-Chloro-o-tolyloxy)butyric acid
Use	Herbicide.

MNO

LC50 values to crustaceans, mg/l	> 40 act, Daphnia pulex (Nishiuchi & Hashimoto 1967)
LC50 values to fishes, mg/l	> 10 48hr, Cyprinus carpio (Nishiuchi & Hashimoto 1967)
Other information about water organisms	LOEC 10 mg/l, Colpidium campylum (Dive et al. 1980).

1276 • Mefluidide

53780-34-0

Synonyms	5'-(Trifluoromethanesulfonamido)acet-2',4'-xylidide
Use	Herbicide; plant growth regulator.
LC50 values to fishes, mg/l	> 100 96hr, Salmo gairdneri Lepomis macrochirus (Pesticide Manual 1983)

1277 • Menadione

58-27-5

LD50 values to birds in oral exposure, mg/kg	> 316 orl-Agelaius phoeniceus (Schafer et al. 1983)
LC50 values to fishes, mg/l	1.2 1d, Ictalurus punctatus 0.92 2d, Ictalurus punctatus 0.785 3d, Ictalurus punctatus 0.72 4d, Ictalurus punctatus (Andaya & Di Giulio 1987)
Effects on the physiology of water organisms	Ictalurus punctatus, 0.185 mg/l, 2 d, hematological effect (change in various blood parameters such as red blood cell count, hematocrit, and serum osmolarity) (Andaya & Di Giulio 1987).

1278 • 1,4-p-Menthadiene

99-85-4

Sumformula of the chemical	C10H16
EINECS-number	2027946
Water solubility, mg/l	< 100 (MITI 1992)
Melting point, °C	-10 (MITI 1992)
Boiling point, °C	183 (MITI 1992)
Total degradation in water	Biodegradation: 89–102% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

1279 • Menthol

89-78-1
15356-70-4
2216-51-5

Synonyms	p-Menthan-3-ol (CAS 89-78-1) DL-Menthol (CAS 15356-70-4) (L)-Menthol (CAS 2216-51-5)

Sumformula of the chemical	C10H200
Water solubility, mg/l	490 (MITI 1992)
Melting point, °C	35–36 (MITI 1992)
Boiling point, °C	103–105 16 mmHg (MITI 1992)
Log octanol/water coefficient, log Pow	3.3 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.5–15 6w, Cyprinus carpio, conc 0.2 mg/l < 4.6–11 6w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	26 48hr, Oryzias latipes (MITI 1992)

1280 • 2-Mercapto benzothiazole 149-30-4

Melting point, °C	> 173 (MITI 1992)
Total degradation in water	Biodegradation: 2.5% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Bioconcentration factor, fishes	< 0.8 6w, Cyprinus carpio, conc 0.1 mg/l < 8 6w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	8.4 48hr Oryzias latipes (MITI 1992)

1281 • 2-Mercapto imidazoline 872-35-5

Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).

1282 • 2-Mercaptobenzimidazole 583-39-1

Sumformula of the chemical	C7H6N2S
Melting point, °C	301–302 (MITI 1992)

MNO

Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	0.7–3.5 6w, Cyprinus carpio, conc 0.5 mg/l < 2.6 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
LC50 values to fishes, mg/l	160 48hr, Oryzias latipes (MITI 1992)

1283 • Mercaptothiazoline 96-53-7

Other information about mammals	LDfr = 20.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

1284 • Mercuric(I) chloride 7546-30-7

Molecular weight	236.04
LD50 values to mammals in oral exposure, mg/kg	210 orl-rat (Lewis & Sweet 1984)
LOEC values to algae, mg/l	0.07 rpd, act, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
LC50 values to fishes, mg/l	0.015–0.184 96hr, Labeo rohita (Deshmukh & Marathe 1980) 0.03–0.054 96hr, Poecilia reticulata (Deshmukh & Marathe 1980) 0.4 24hr, Carassius auratus (Sharma & Davis 1980) 0.18 96hr, Gambusia affinis (Joshi & Rege 1980)

1285 • Mercuric(II) chloride 7487-94-7

Synonyms	Mercury bichloride Mercury chloride
Sumformula of the chemical	$HgCl_2$
Use	Manufacture of calomel and other mercury compounds, disinfectant, organic synthesis, analytical reagent, metallurgy, tanning, catalyst for vinyl chloride, sterilant for seed potatoes; fungicide, insecticide, and wood preservative; embalming fluids, textile printing, dry batteries, photography, process engraving and lithography.
State and appearance	White crystals or powder, odourless.
Molecular weight	271.49
Melting point, °C	276
Boiling point, °C	303
Mobility	Transformation to methylmercury is the most important part of Hg cycle in the environment. Hg is strongly bound to organic matter is soil and sediment. – Inorganic Hg compounds are methylized abiotically in the presence of methylcobalamine (B12-CH3) and biotically with help of enzymes ($Hg^{2+} \rightarrow CH_3Hg^+$ + / $(CH_3)_2Hg$) (Kaiser & Tölg 1980).
Other information about degradation	Organic Hg compounds kan be formed and break up chemically, biochemically and through photosynthesis as well in atmosphere as in aquatic environment: $CH_3Hg^+ \leftrightarrow (CH_3)_2Hg \leftrightarrow Hg \leftrightarrow Hg^{2+}$ (Anon. 1989).

MNO

Metabolism in mammals	Inorganic Hg is mainly stored in kidneys (WHO 1976). Organic Hg compounds decompose to inorganic Hg and accumulates in kidneys (WHO 1976). Methylmercury is absorbed in alimentary canal 90–100% after intake with food, whereas inorganic Hg is absorbed less than 15% (WHO 1976). Brains seem to be very sensitive to methylmercury and for Hg vapour (Berlin 1986). Methylmercury is very slowly decombosed mainly through faeces (Berlin 1986).	
LD50 values to mammals in oral exposure, mg/kg	1 37 10	orl-rat (Lewis & Sweet 1984) orl-rat (Pomeroy et al. 1980) orl-rat (Lewis & Tatken 1979)
LDLo values to mammals in oral exposure, mg/kg	29	orl-hmn (Lewis & Sweet 1984)
LDLo values to mammals in non-oral exposure, mg/kg	345	skn-gpg (Lewis & Sweet 1984)
LCLo values to mammals in inhalation exposure, mg/kg	300	10min, ihl-mus (Lewis & Sweet 1984)
Health effects	Inorganic bivalent Hg compounds and unstabile organic Hg compounds induce damages in kidneys (Berlin 1986). Methylmercury has effects on the central nervous system – motoric and mental disorders etc. (Berlin 1986).	
LDLo values to birds in oral exposure, mg/kg	2200	orl-pgn (Lewis & Sweet 1984)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 0.01 mg/l (Bringmann & Kühn 1980a)	
NOEC values to algae, mg/l	0.08	rpd, schr, Selenastrum capricornutum (Slooff et al. 1983)
LC50 values to crustaceans, mg/l	0.003 0.0031 0.0032	48hr, Daphnia pulex 48hr, Daphnia magna 48hr, Daphnia cucullata (Canton & Adema 1978)
	0.095	96hr, Macrobrachium lamarrei (Murti & Shukla 1984)
	0.0094 0.0038	1d, Daphnia magna 2d, Daphnia magna (Khangarot et al. 1987)
	0.140–0.790	4d, Procambarus clarkii (Del Ramo et al. 1987)
	0.2 0.01	48hr, Asellus aquaticus (Slooff 1983) 48hr, Gammarus pulex (Slooff 1983)
	0.0029	Ceriodaphnia (Elnabarawy et al. 1986)
	0.005	48hr, Daphnia (Biesinger & Christensen 1972)
	3.3–10	48hr, Crangon (Portmann & Wilson 1971)
EC50 values to crustaceans, mg/l	0.65 0.199 0.47 0.001	mbt, 2 d, Asellus aquaticus mbt, 4 d, Asellus aquaticus mbt, 2 d, Crangonyx pseudogracilis mbt, 4 d, Crangonyx pseudogracilis (Martin & Holdich 1986)
	0.0081 0.0052	mbt, 1d, Daphnia magna mbt, 2d, Daphnia magna (Khangarot & Ray 1987)

MNO

LC50 values to fishes, mg/l	0.65 0.05	48hr, Salmo gairdneri 48hr, Pimephales promelas (Slooff et al. 1983)
	0.16	96hr, static, Lepomis macrochirus (Holcombe et al. 1983)
	0.37	1 d, Catla catla (Rai 1987)
	0.98 0.63	1d, Lepidocephalus thermalis 4d, Lepidocephalus thermalis (Victor et al. 1986)
	700	28d, Neanthes arenaceodentata, juv. (Christensen 1975)
	0.1	28d, Capitetta capitata (Reish et al. 1976)
Effects on the physiology of water organisms	Catla catla, 0.370 mg/l, 1 d, biochemical effect (change in physiochemical process including glycogen uptake, cholesterol levels and lipid analysis) (Rai 1987). Chara vulgaris, 0.000001 M, 7 d, measurable change in length and/or weight (Heumann 1987). Cyprinus carpio, 0.200 mg/l, change in rate of ingestion or fecal pellet production (Muthukrishnan et al. 1986). Lepidocephalus thermalis, 0.070 mg/l, 10 d, histological effect (presence of physical damage to tissues) (Victor et al. 1986).	
Other information about water organisms	LC50, 96hr, 0.37 mg/l, gastropod (Holcombe et al. 1983). Chara vulgaris, 0.000001 M, 7 d, 100% mortality including algicidal and herbicidal effects (Heumann 1987). LC50, 48hr, 0.18 mg/l, Tubificidae LC50, 48hr, 0.55 mg/l, Chironomus gr. thummi LC50, 48hr, 0.32 mg/l, Erpobdella octoculata LC50, 48hr, 0.61 mg/l, Lymnaea stagnalis LC50, 48hr, 0.075 mg/l, Dugesia cf. lugubris LC50, 48hr, 0.076 mg/l, Hydra oligactis LC50, 48hr, 0.22 mg/l, Corixa punctata LC50, 48hr, 10.3 mg/l, Ischura elegans LC50, 48hr, 0.17 mg/l, Nemoura cinerea LC50, 48hr, 0.05 mg/l, Cloeon dipterum (Slooff 1983) LC50, 96hr, 0.37 mg/l, static, Aplexa hypnorum (Holcombe et al. 1983) Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 0.07 mg/l protozoa (Entosiphon sulcatum): 0.018 mg/l (Bringmann & Kühn 1980a) EC0, Microcystis aeruginosa, 0.05 mg/l (DABAWAS 1982). Phytoplankton, marine, pht, 0.001 mg/l (Knauer & Martin 1972). Daphnia, rpd, 0.0034 mg/l (Biesinger & Christensen 1972).	

MNO

1286 • Mercuric oxide 21908-53-2

Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Other information about bioaccumulation	Confirmed to be accumulated on a high level (Anon. 1987).

1287 • Mercuric thiocyanate 592-85-8

LC50 values to crustaceans, mg/l	0.09	96hr, Palaemonetes pugio (Verschueren 1983)
LC50 values to fishes, mg/l	0.15	96hr, Pimephales promelas (Verschueren 1983)

1288 • Mercury compounds

7439-97-6

Sumformula of the chemical	Hg
Molecular weight	200.61
Density, kg/m³	13595 0 °C
Vapour pressure, mmHg	0.0012
Water solubility, mg/l	60 20 °C
Melting point, °C	-38.86
Boiling point, °C	357.3
Mobility	Transformation to methylmercury is the most important part of Hg cycle in the environment. Hg is strongly bound to organic matter is soil and sediment. – Inorganic Hg compounds are methylized abiotically in the presence of methylcobalamine (B12-CH3) and biotically with help of enzymes ($Hg2+ \rightarrow CH3Hg+ + /$ (CH3)2Hg) (Kaiser & Tölg 1980).
Other information about degradation	Organic Hg compounds can be formed and break up chemically, biochemically and through photosynthesis as well in atmosphere as in aquatic environment: $CH3Hg+ \leftrightarrow (CH3)2Hg \leftrightarrow Hg \leftrightarrow Hg2+$ (Anon. 1989)
Metabolism in mammals	Inorganic Hg is mainly stored in kidneys (WHO 1976). Organic Hg compounds decompose to inorganic Hg and accumulates in kidneys (WHO 1976). Methylmercury is absorbed in alimentary canal 90–100% after intake with food, whereas inorganic Hg is absorbed less than 15% (WHO 1976). Brains seem to be very sensitive to methylmercury and for Hg vapour (Berlin 1986). Methylmercury is very slowly decomposed mainly through faeces (Berlin 1986).
Bioconcentration factor, fishes	1–6 fish (Perwak et al. 1985)
LD50 values to mammals in oral exposure, mg/kg	500 orl-rat, inorg.Hg (Kaiser & Tölg 1980)
LC50 values to mammals in inhalation exposure, mg/m³	29 30hr, ihl-rbt (Lewis & Sweet 1984)
TCLo values to mammals in inhalation exposure, mg/kg	0.15 46d, ihl-wmn (Lewis & Sweet 1984)
Effects on the physiology of mammals	Cat, inhalation, > 0.010 mg/m³ Hg vapour in air, effects on reflexes (Nordberg 1981). Rat, inhalation, NOEC, 0.003 mg/m³, Hg vapour (Nordberg 1981).
Other information about mammals	Toxic when 5 mg/kg in brains and in muscles of mink. Harp seal was killed at 25 mg/kg in 20–26 days (Virtanen & Nuuja 1987).
Health effects	Inorganic bivalent Hg compounds and unstabile organic Hg compounds induce damages in kidneys (Berlin 1986). Methylmercury has effects on the central nervous system – motoric and mental disorders etc. (Berlin 1986).
Carcinogenicity	Classification: Group D: not enough evidence in animal experiments (USEPA 1986).
Mutagenicity	Drosophila: slight mutagenicity (Perwak et al. 1985).
Teratogenicity	Teratogenic effects on fish and birds (Leonard et al. 1983).
Effects on amphibia	LC50 0.051 ppm, 96hr, tadpoles of Rana hexadactyla (Khangarot et al. 1985).

Effects on plants	The 4-leaf stage plants (Pennisetum typhoideum, Medicago sativa, Abelmoschus esculentum) were grown for 24 hours in Knop's nutrient solution mixed with a known concentration (1ppb, 10 ppb,...) of Hg solutions (HgCl2). Subtle damage in terms of reduced chlorophyll content and reduction in standing phytomass of the plants was observed at 1 ppb and visible foliar symptoms at 10 ppb (Mhatre & Chaphekar 1984). When the roots of onion bulbs had reached a length of about 15 mm the bulbs were transferred to glas jars containing the experimental solution, where they were kept for 72 hours: Lowest lethal dose for Allium cepa roots 1.Panogen 5 0.00125 mol/l (250 ppm Hg) 2.Panogen 8 0.00032 mol/l (64 ppm Hg) 3.Methyl mercury dicyanidamide 0.00025 mol/l (50 ppm Hg) 4.Methyl mercury hydroxide 0.00025 (50 ppm Hg) Lowest C-mitotic dose 1. 0.00000025 mol/l (0.05 ppm Hg) 2. 0.00000080 mol/l (0.16 ppm Hg) 3. 0.00000060 mol/l (0.13 ppm Hg) 4. 0.00000025 mol/l (0.05 ppm Hg) 5.Phenyl mercury hydroxide 0.00000080 mol/l (0.16 ppm Hg) 6.Methoxyethyl mercury chloride 0.0000314 mol/l (0.63 ppm) Hg) (Ramel 1969).
LC50 values to crustaceans, mg/l	0.65 Hg(II),48hr, mbt, Asellus aquaticus 0.199 Hg(II),96hr, mbt, Asellus aquaticus (Martin & Holdich 1986) 0.013 21d, Daphnia magna 0.005 48hr, without food, D.magna (Biesinger & Christensen 1972) 0.15 Hg(II), 96hr, Gammarus duebeni (Inman & Lockwood 1977) 0.12 Hg(II), 96hr, Gammarus duebeni (Moulder 1980) 0.03–0.10 Hg(II), Gammarus (Jung 1975) 0.006–0.020 48hr, Daphnia magna (Barera & Adams 1983)
EC50 values to crustaceans, mg/l	0.006–0.0248hr, Daphnia magna (Barera & Adams 1983) 0.0052 48hr, mbt, Daphnia magna (Khangarot & Ray 1987) 0.0067 21 d, rpd, Daphnia magna (Biesinger & Christensen 1972)
LOEC values to crustaceans, mg/l	0.0034 21 d, Daphnia magna, HgCl2 (Biesinger & Christensen 1972)
LC50 values to fishes, mg/l	0.16 96hr, Lepomis macrochirus (Holcombe et al. 1983) 0.9 96hr, Channa punctata (Saxena & Parashari 1983) 0.0078–0.134 96hr, Barbus conchonius (Gill & Pant 1981) 0.168 96hr, Pimephales promelas (Snarski & Olson 1982) 0.005 28 d, Salmo gairdneri (Birge et al. 1980)
LOEC values to fishes, mg/l	0.00026 rpd, grw, chr, Pimephales promelas (Snarski & Olson 1982)
Other information about water organisms	LC50 0.36 mg/l, 96hr, Aplexa hypnorum (Holcombe et al. 1983). LC50 0.023 mg/l, 96hr, Lymnea acuminata (Khangarot et al. 1982). LC50 0.16 mg/l, 96hr, Nais communis; LC50 0.29 mg/l, 96hr, Ilyodrilus frantzi (Chapman & Mitshell 1986).

1289 • Mertect * 148-79-8

Active ingredients	Thiabendazole * 450 g/l	
Use	Fungicide.	
LC50 values to crustaceans, mg/l	24	96hr, Nitocra spinipes (Linden et al. 1979)

1290 • Mesityl oxide 141-79-7

Synonyms	4-Methyl-3-pentene-2-one Isopropylidene acetone Isobutenyl methyl ketone Methyl isobutenyl ketone 2-Methyl-2-penten-4-one	
Sumformula of the chemical	C6H10O	
Odour	Quality: sweet Hedonic tone: pleasant Threshold odour concentration absolute: 0.017 ppm 50% recognition: 0.051 ppm 100% recognition: 0.051 ppm Odour index 100% recognition: 210 000 (Hellman & Small 1974).	
Molecular weight	98.16	
Melting point, °C	-59	(MITI 1992)
Boiling point, °C	129.5	760 mmHg (MITI 1992)
Chemical oxygen demand, g O2/g	2.4	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g O2/g	1.91	5 days (Bridie et al. 1979)
Total degradation in water	Biodegradaation: 77.2% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	710 1120	orl-mus orl-rat (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	354 5150	ipr-mus skn-rbt (Sweet 1987)
LC50 values to mammals in inhalation exposure, mg/m³	10000 9000	ihl-mus, 2hr ihl-rat, 4hr (Sweet 1987)
LDLo values to mammals in non-oral exposure, mg/kg	840	scu-rbt (Sweet 1987)
TCLo values to mammals in inhalation exposure, ppm	25	ihl-hmn (Sweet 1987)

MNO

Other information about mammals	Skin and eye irritation data: eye, human, 25 ppm, 15 min; skin, rabbit, 430 mg open, mild; eye, rabbit 4.325 mg, severe (Sweet 1987).
Effects on amphibia	LDLo, 1400 mg/kg, scu-frog (Sweet 1987).
LC50 values to fishes, mg/l	540 24hr, Carassius auratus (Bridie et al. 1979)

1291 • Mesitylene 108-67-8

Synonyms	1,3,5-Trimethylbenzene
Sumformula of the chemical	C9H12
Water solubility, mg/l	< 10 (MITI 1992)
Melting point, °C	-51.7– -44.8 (MITI 1992)
Boiling point, °C	164.7 (MITI 1992)
Log octanol/water coefficient, log Pow	3.6 (Schwarzenbach & Westall 1981) 3.42 (Sangster 1989) 3.93 (MITI 1992)
Log soil sorption coefficient, log Kom	2.82 observed (Sabljic 1987) 2.75 calculated (Sabljic 1987)
Henry's law constant, Pa x m^3/mol	803.2 calc. (Yaws et al. 1991)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	23–342 10w, Cyprinus carpio, conc 0.15 mg/l 42–328 10w, Cyprinus carpio, conc 0.015 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987) (1,3,5-trimethylbenzene).
LC50 values to fishes, mg/l	13 96hr, Carassius auratus (Brenniman et al. 1976) 8.6 48hr, Oryzias latipes (MITI 1992)

1292 • Metallyl chloride 563-47-3

Water solubility, mg/l	1.4 (MITI 1992)
Melting point, °C	< -30 (MITI 1992)
Boiling point, °C	73 (MITI 1992)
Chemical oxygen demand, g 02/g	1.18 5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.81 5 days (Bridie et al. 1979)

MNO

Total degradation in water	Biodegradation: 89–107% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).	
LC50 values to fishes, mg/l	14	24hr, Carassius auratus (Bridie et al. 1979)

1293 • Metamitron

41394-05-2

Synonyms	4-Amino-3-methyl-6-phenyl-1,2,4-triazin-5(4H)-one(C–A) 4-Amino-4,5-dihydro-3-methyl-6-phenyl-1,2,4-triazin-5-one	
Sumformula of the chemical	C10H10N4O	
Purity, %	98	/w
Use	Active ingredient in herbicides.	
State and appearance	Solid, crystalline, colourless to bright yellow.	
Molecular weight	202	
Water solubility, mg/l	1820	
Melting point, °C	167–169	
Effects on plants	The roots of maize (Zea mays L.) and 7 other plant species were exposed to 5 x 10–6 mol/l metamitron in the nutrient solution which led to inhibition of photosynthesis (van Oorschot & van Leeuwen 1979).	
LC50 values to fishes, mg/l	> 100	96hr, Carassius auratus (Pesticide Manual 1983)

1294 • Metasystox

8022-00-2

LC50 values to crustaceans, mg/l	1.567 1.438 1.336	1d, Macrobrachium lamarrei 2d, Macrobrachium lamarrei 3d, Macrobrachium lamarrei (Mary et al. 1986)

1295 • Metazol D3T *

73482-04-9

Active ingredients	Dazomet * 21%; Benzothiazolethiol * 6%	
Use	Herbicide; slimicide.	
LC50 values to crustaceans, mg/l	0.54	96hr, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	14	96hr, Alburnus alburnus (Linden et al. 1979)

1296 • Methamidophos

10265-92-6

Other information about mammals	LDfr = 77.8 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).	
LC50 values to fishes, mg/l	68	96hr, juv., Cyprinus carpio (Chin & Sudderuddin 1979)

MNO

1297 • Methanesulfonylchloride 3518-65-8

LC50 values to fishes, mg/l	11 15	96hr, Lepomis macrochirus 96hr, Menidia audens (Dawson et al. 1977)

1298 • Methanol 67-56-1

Synonyms	Methyl alcohol	
Sumformula of the chemical	CH4O	
Use	Solvent.	
Odour	Quality: sour, sharp Hedonic tone: neutral Threshold odour concentration absolute: 4.26 ppm 50% recognition: 53.3 ppm 100% recognition: 53.3 ppm Odour index 100% recognition: 2 393 (Hellman & Small 1974).	
Molecular weight	32.04	
Vapour pressure, mmHg	92	at 20 °C (Weber et al. 1981)
Water solubility, mg/l	Infinite 36310	 (Leahy 1986)
Melting point, °C	-97.8	(Suntio et al. 1988)
Boiling point, °C	64.7	at 760 mmHg
Log octanol/water coefficient, log Pow	-0.7 -0.77 -0.74	(Leahy 1986) (Hansch & Leo 1985) (Sangster 1989)
Henry's law constant, Pa x m³/mol	11.03 13.68	calc. (Suntio et al. 1988) (Snider & Dawson 1985)
Volatilization	Relative volatility (nBuAc=1) = 5.90 The value of Henry's law constant indicates that volatilization from environmental waters may be significant (Lyman et al. 1982). The volatilization half-life from a model river has been estimated to be 5.3hr (Lyman et al. 1982). The volatilization half-life from an environmental pond has been estimated to be 2.6 days (USEPA 1987).	
Mobility	Methanol is miscibility in water and low octanol/water partition coefficient suggest high mobility in soil (Howard 1990). Miscible (Merck Index 1983).	
Photochemical degradation in air	Methanol is expected to exist almost entirely in the vapour phase in the ambient atmosphere, based on its vapour pressure. It is degraded by reaction with photochemically produced hydroxyl radicals with estimated half-life 17.8 days in a typical ambient atmosphere. Atmospheric methanol can also react with nitrogen dioxide in polluted air to yield methyl nitrite (Howard 1990).	
Photochemical degradation in soil	Sediment an clay suspensions solution did not photocatalyze the degradation of methanol in aqueous solution during irradiation with UV light (Oliver et al. 1979).	
Photochemical degradation in water	Methanol in aqueous solution exhibited no degradation when exposed to sunlight using an EPA test protocol (Hustert et al. 1981).	

Total degradation in soil	Methanol is expected to be significantly biodegradable in soil based on the results of a large number of biological screening studies, which include soil microcosm studies (Howard 1990).	
Other information about degradation	Standard dilution BOD water, 5-day 48% BODT, sewage inocula (Dore et al. 1975). Standard dilution BOD water, 5-day 76% BODT, 20day 97% BODT, sewage inocula (Price et al. 1974). Respirometric dilution, 5-day 82.9% BODT, sewage inocula (Wagner 1976). Anaerobic-water, 75-80% degradation, sewage inocula (Bekes et al. 1975). Biological treatment simulation, 80% degradation, adapted activated sludge (Swain 1978). Standard dilution, 5-day 88.7% BODT; seawater dilution, 5-day 70.7% BODT (Takemoto et al. 1981). Soil-sediment suspensions, aerobic conditions, 5-day CO2 evolution (14-C) of 53.4%; soil-sediment suspensions, anaerobic conditions, 5-day CO2 evolution (14-C) of 46.3% (Scheunert et al. 1987).	
Other information about bioaccumulation	The BCF of methanol experimentally measured in fish (golden ide) was less than 10 (Freitag et al. 1985). Based on the octanol/water partition coefficient, the BCH value for methanol can be estimated to be 0.2 from a recommended regression-derived equation (Lyman et al. 1982).	
LD50 values to mammals in oral exposure, mg/kg	13000	orl-rat
Maximum longterm immission concentration in air for plants, mg/m³	15	VDI 2306
Maximum longterm immission concentration in air for plants, ppm	10	VDI 2306
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 6600 mg/l (Bringmann & Kühn 1980a).	
EC50 values to microorganism, mg/l	42000 158000 90147	15 min Microtox (Hermens et al. 1985) Microtox (Green et al. 1985) Biodegradation inhibition (Vaishnav 1986)
LOEC values to algae, mg/l	530	rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to crustaceans, mg/l	12000	96hr, 21 °C, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	8000 28100 > 28000	48hr, Salmo trutta (Price et al. 1974) 96hr, Pimephales promelas (Veith et al. 1983) 96hr, 10 °C, Alburnus alburnus (Linden et al. 1979)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 8000 mg/l protozoa (Entosiphon sulcatum): > 10000 mg/l (Bringmann & Kühn 1980a).	

1299 • Methidathion 950-37-8

Effects on the physiology of water organisms	Cyprinus carpio, 2 mg/l, 1 d, change in enzyme activity (Vig et al. 1987).

1300 • Methiocarb

2032-65-7

Synonyms	3,5-Dimethyl-4-methylthiophenylmethylcarbamate 4-Methylthio-3,5-xylyl methylcarbamate Mercaptodimethur	
Use	Insecticide, acaricide; active ingredient in molluscicides.	
Molecular weight	225.33	
Melting point, °C	121	
Log soil sorption coefficient, log Kom	2.08	(Sabljic 1987)
Total degradation in water	0% of original compound found after 1 week in river water (initial concentration 10 μg/l) (Verschueren 1983).	
LD50 values to mammals in oral exposure, mg/kg	15	orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	350	skn-rat (Lewis & Sweet 1984)
Other information about mammals	ALD = 8.0 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987).	
LD50 values to birds in oral exposure, mg/kg	5	orl-bwd (Lewis & Sweet 1984)
	4.67–12.6	orl-Agelaius phoeniceus
	11.3–50.0	orl-Sturnus vulgaris
	8.84–10.4	orl-Coturnix coturnix
	17.8	orl-Passer domesticus
	10	orl-Quiscalus quiscula
	13.3	orl-Columba livia
	2.37–3.00	orl-Carbodacus mexicanus
	13.3	orl-Anas platyrhynchos
	13.3–1000	orl-Phasianus colchicus
	3.16	orl-Xanthocephalus xanthocephalus
	7.5	orl-Molothrus ater
	4.22	orl-Cassidix major
	1.33	orl-Melopsittacus undulatus
	19.6–24.0	orl-Colinus virginianus
	7.5	orl-Corvus brachyrhynchos
	5.62	orl-Bombycilla cedrorum
	3.16	orl-Zebauda auriculata
	3.16	orl-Zonotrichia atricapilla
	5.62	orl-Passer luteus
	4.22	orl-Eremophila alpestris
	4.22	orl-Scardafella inca
	10	orl-Zenaida macroura
	4.87–7.50	orl-Ploceus taeniopterus
	10	orl-Zenaida asiatica
	5.62–7.50	orl-Euplectes orix
	4.22–7.50	orl-Larus delawaresis
	23.7	orl-Grus canadensis
	5.62	orl-Agelaius tricolor
	24	orl-Loportyx californica
	7.5	orl-Ploceus cucullatus
	4.22	orl-Zonotrichia leucophrys (Schafer et al. 1983)
LD50 values to birds in dermal exposure, mg/kg	100	skn-bwd (Lewis & Sweet 1984)

MNO

LC50 values to fishes, mg/l	1–10 0.64	96hr, Cyprinus carpio 96hr, Salmo gairdneri (Pesticide Manual 1983)
	0.11 0.64	act, Lepomis macrochirus act, Salmo gairdneri (Kenaga 1979)

1301 • Methomyl

16752-77-5

Synonyms	N-((Methylcarbamoyl)oxy)thioacetimidic acid methylester	
Products containing the chemical	Insecticide 1 Insecticide 179 Lannate Mesomile	
Use	Insecticide.	
Molecular weight	162.23	
Log soil sorption coefficient, log Kom	2.2	(Sabljic 1987)
LD50 values to mammals in oral exposure, mg/kg	17 10	orl-rat (Lewis & Sweet 1984) orl-mus (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	5880	skn-rbt (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	10 15	orl-bwd orl-dck (Lewis & Sweet 1984)
	10 13.3–42.2 23.7 13.3–31.6 13.3–23.7 10	orl-Agelaius phoeniceus orl-Sturnus vulgaris orl-Coturnix coturnix orl-Passer domesticus orl-Quiscalus quiscula orl-Columba livia (Schafer et al. 1983)
Effects on plants	Methomyl insecticide (Lannate 90 wp) was selectively phytotoxic on hydrids and inbreds of sweet corn (Zea mays) having the Texas male sterile cytoplasm. In field and greenhouse tests, phytotoxicity was visible at leaf tips and margins 2 days after a foliar application of 300 ppm methomyl. In the greenhouse a pre- and postemergence application of methomyl, 75 mg/kg soil resulted in severe necrosis, chlorosis, and eventual death of the seedlings (Humaydan & Scott 1977).	
LC50 values to crustaceans, mg/l	0.045	ct, Daphnia pulex (Hashimoto & Nishiuchi 1981)
NOEC values to crustaceans, mg/l	0.0037	rpd, schr, Daphnia magna (Macek & Sleight 1977)
LC50 values to fishes, mg/l	3.4 0.87	96hr, Salmo gairdneri 96hr, Lepomis macrochirus (Pesticide Manual 1983)
	2.8 2.7	48hr, Cyprinus carpio 48hr, Carassius auratus (Hashimoto & Nishiuchi 1981)
NOEC values to fishes, mg/l	0.375	rpd, chr, Pimephales promelas (Macek & Sleight 1977)

MNO

1302 • Methoprene 40596-69-8

Synonyms	Altosid-SR-10 ZR-515 (Isopropyl(2E-4E)-11-methoxy-3,7,11-trimethyl-dodeca-2,4-dienoate
Use	Insect growth regulator; prevents adult emergence of mosquitoes, houseflies, stable-flies and blackflies by preventing metamorphosis of final instar larvae.
State and appearance	Amber liquid.
Specific gravity (water=1)	0.9261 at 20 °C
Vapour pressure, mmHg	0.0000237 at 25 °C 0.00016 at 40 °C
LD50 values to mammals in oral exposure, mg/kg	34600 orl-rat (Martin 1968)
LD50 values to mammals in non-oral exposure, mg/kg	3000 skn-rbt (Martin 1968)
Teratogenicity	Teratogenicity: no effects on rats at 1000 mg/kg (Martin 1968).
LC50 values to crustaceans, mg/l	2.15 adult female,96hr, Gammarus aequieaudu 1.95 adult male,96hr, Gammarus aequieaudu (Gradon et al. 1976)
LC50 values to fishes, mg/l	106 96hr, Salmo gairdneri 86 96hr, Oncorhynchus kisutch (McKague & Pridmore 1978) 4.39 act, Salmo trutta (Martin 1968)
Effects on the reproduction of water organisms	Decapod: Rhithropanopeus harrissii: adult: 1.30 mg/l, 12–15 days. Progressive inhibition of vitellogenesis and stimulation of spermatogenesis after 30–45 days (Payen & Costlow 1977).

1303 • 3-Methoxy nitrobenzene 555-03-3

Synonyms	m-Nitroanisole
Water solubility, mg/l	< 500 (MITI 1992)
Melting point, °C	38–39 (MITI 1992)
Boiling point, °C	258 (MITI 1992)
Total degradation in water	Biodegradation: 1% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	2.4–4.3 6w, Cyprinus carpio, conc 0.05 mg/l 2.5–9 6w, Cyprinus carpio, conc 0.005 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	83 48hr, Oryzias latipes (MITI 1992)

MNO

1304 • 1-Methoxy-2-hydroxypropane 107-98-2

Sumformula of the chemical	C4H10O2
EINECS-number	2035391
Water solubility, mg/l	> 100000 (MITI 1992)
Melting point, °C	< -10 (MITI 1992)
Boiling point, °C	118.8–121.0 (MITI 1992)
Total degradation in water	Biodegradation: 88.92% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

1305 • 4-Methoxy-4-methyl-2-pentanone 107-70-0

Chemical oxygen demand, g O2/g	2.24	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g O2/g	0.11	5 days (Bridie et al. 1979)
LC50 values to fishes, mg/l	3800	24hr, Carassius auratus (Anon. 1975)

1306 • 3-Methoxy-n-butanol 2517-43-3

Sumformula of the chemical	C5H12O2
Melting point, °C	-85 (MITI 1992)
Boiling point, °C	160 760 mmHg (MITI 1992)
Total degradation in water	Biodegradation: 83.8% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

1307 • 3-Methoxy-n-butyl acetate 4435-53-4

Synonyms	1-Butanol, 3-methoxy-, acetate Acetic acid, 3-methoxybutyl ester
Sumformula of the chemical	C7H14O3
EINECS-number	2246449
Water solubility, mg/l	4600 (20°C) (MITI 1992)
Boiling point, °C	172.5 760 mmHg (MITI 1992)

MNO

Total degradation in water	Biodegradation: 63.5% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

1308 • 4-Methoxy-tert-butyl phenol 121-00-6

Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).

1309 • 4-Methoxyacetanilide 51-66-1

Sumformula of the chemical	C9H11NO2	
Log soil sorption coefficient, log Kom	1.16	(Sabljic 1987)

1310 • 2-Methoxyaniline 90-04-0

Synonyms	o-Anisidine 2-Aminoanisole	
Molecular weight	125.15	
Specific gravity (water=1)	1.0923	at 20/4 °C
Vapour density (air=1)	4.25	
Conversion factor, 1 ppm in air=	5.12	mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.2	ppm
Vapour pressure, mmHg	< 0.1	mmHg at 30 °C
Melting point, °C	5	(MITI 1992)
Boiling point, °C	225	(MITI 1992)
Log octanol/water coefficient, log Pow	0.95	
Total degradation in soil	Decomposition period by a soil micro flora: > 64 days (Verschueren 1983).	
Total degradation in water	Biodegradation: 40–69% by BOD (on the upward trend) period: 14d substance: 100mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LD50 values to birds in oral exposure, mg/kg	750 > 1000 422 421	orl-Agelaius phoeniceus orl-Sturnus vulgaris orl-Coturnix coturnix orl-Passer domesticus (Schafer et al. 1983)

MNO

Effects on wastewater treatment	Degradation by Aerobacter: 500 mg/l at 30 °C: ring disruption: parent: 92% in 120hr mutant: 100% in 16hr (Verschueren 1983).

1311 • 4-Methoxyaniline 104-94-9

Synonyms	p-Anisidine p-Aminoanisole p-Aminomethoxybenzene p-Aminomethylphenylether	
Molecular weight	123.15	
Specific gravity (water=1)	1.0605	at 67/4 °C
Vapour density (air=1)	4.25	
Conversion factor, 1 ppm in air=	5.12	mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.2	ppm
Melting point, °C	57	(MITI 1992)
Boiling point, °C	246	(MITI 1992)
Log octanol/water coefficient, log Pow	0.95	
Total degradation in soil	Decomposition period by a soil micro flora: 64 days (Verschueren 1983).	
Total degradation in water	Biodegradation: 65.3% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LD50 values to birds in oral exposure, mg/kg	316 316–1000 > 1000	orl-Agelaius phoeniceus orl-Sturnus vulgaris orl-Coturnix coturnix (Schafer et al. 1983)
Effects on wastewater treatment	Degradation by Aerobacter: 500 mg/l at 30 °C: ring disruption: parent: 86% in 120hr mutant: 100% in 12hr (Verschueren 1983).	

1312 • Methoxychlor 72-43-5

Synonyms	Methoxy-DDT 1,1,1-Trichloro-2,2-di(4-methoxyphenyl)ethane	
Use	Insecticide.	
Molecular weight	345.66	
Water solubility, mg/l	0.04	24 °C
Melting point, °C	98	

MNO

Log octanol/water coefficient, log Pow	4.3	(Mackay 1982)
LD50 values to mammals in oral exposure, mg/kg	5000 1850	orl-rat orl-mus (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	7600	skn-rat (Lewis & Sweet 1984)
TDLo values to mammals in non-oral exposure, mg/kg	2414	skn-hmn (Lewis & Sweet 1984)
Carcinogenicity	NCI carcinogenesis bioassay completed: results negative; mus, rat (Lewis & Sweet 1984).	
LC50 values to crustaceans, mg/l	0.0005	96hr, Orconectes nais (Sanders 1972)
	0.0008	96hr, Gammarus lacustris (Sanders 1969)
	0.0037	act, Daphnia pulex (Frear & Boyd 1967)
	11.7–13.8	48hr, Daphnia magna (Bogacka et al. 1983)
	0.004	act, Daphnia magna (Kenaga 1979)
EC50 values to crustaceans, mg/l	0.0008	48hr, Daphnia pulex (Shapiro 1979)
LC50 values to fishes, mg/l	0.02 0.06	96hr, Salmo gairdneri 96hr, Lepomis macrochirus (Edwards 1977)
	0.0075 0.02	96hr, Pimephales promelas 96hr, Perca flavescens (Verschueren 1983)
	0.028	96hr, Oncorhynchus tshawytscha (Oseid et al. 1974)
	0.052 0.067	24hr, Salmo gairdneri 24hr, Lepomis macrochirus (Pesticide Manual 1983)
	11.5	48hr, Lebistes reticulatus (Bogacka et al. 1983)
	0.075 0.03 0.009	act, Lepomis macrochirus act, Salmo gairdneri act, Pimephales promelas (Kenaga 1979)
LOEC values to fishes, mg/l	0.023	srv, chr, Cyprinodon variegatus (Ward & Parrish 1980)
	0.023	srv, schr, Cyprinodon variegatus (Parrish et al. 1977)
	0.00013	srv, chr, Pimephales promelas (Merna & Eisele 1973)
NOEC values to fishes, mg/l	0.012	srv, schr, Cyprinodon variegatus (Parrish et al. 1977)

1313 • 1-Methoxynaphthalene 2216-69-5

Water solubility, mg/l	10	(MITI 1992)
Boiling point, °C	256–266	(MITI 1992)
Log octanol/water coefficient, log Pow	3.45	(MITI 1992)

Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	130–259 106–221	8w, Cyprinus carpio, conc 0.02 mg/l 8w, Cyprinus carpio, conc 0.002 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	9.5	48hr, Oryzias latipes (MITI 1992)

1314 • 3-Methoxyphenol 150-19-6

LC50 values to fishes, mg/l	75–77 55–60 8.7	48hr, Pimephales promelas 96hr, Pimephales promelas 192hr, Pimephales promelas (Phipps et al. 1981)

1315 • 4-Methoxyphenol 150-76-5

Synonyms	Hydroquinone monomethyl ether p-Hydroxyanisole	
Sumformula of the chemical	C7H8O2	
Use	Manufacture of antioxidants, pharmaceuticals, plasticizers, dyestuffs; stabilizer for chlorinated hydrocarbons and ethyl cellulose, inhibitor for acrylic monomers and acrylonitriles, UV inhibitor.	
State and appearance	White, waxy solid.	
Specific gravity (water=1)	1.55	20/20 °C
Water solubility, mg/l	40	(MITI 1992)
Melting point, °C	55–58	(MITI 1992)
Boiling point, °C	243	
Log octanol/water coefficient, log Pow	1.34	Anon. 1986
Other physicochemical properties	Slightly soluble in water; readily soluble in benzene, acetone ethanol, ethyl acetate. Combustible.	
Total degradation in water	Biodegradation: 79–95% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
LD50 values to birds in oral exposure, mg/kg	> 113	orl-Agelaius phoeniceus (Schafer et al. 1983)
LC50 values to fishes, mg/l	28.6 200	act, Salmo gairdneri (Hodson et al. 1984) 48hr, Carassius auratus (McKee & Wolf 1963)
Other information about water organisms	Tetrahymena pyriformis, EC50, grw, 2 d, 172.4 mg/l (Schultz 1987).	

1316 • 3-(o-Methoxyphenoxy)-1,2-propanediol-1-carbamate 532-03-6

Sumformula of the chemical	C11H15NO5
Water solubility, mg/l	7200 (MITI 1992)
Melting point, °C	92–94 (MITI 1992)
Log octanol/water coefficient, log Pow	0.61 (MITI 1992)
Total degradation in water	Biodegradation: 3–6% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

1317 • 1-(2-Methoxyphenyl)-2-nitroethene 3316-24-3

Other information about mammals	LDfr = 30.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

1318 • 4-(Methoxyphenyl)thiourea 2293-07-4

Other information about mammals	ALD = 12.0 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987).

1319 • Methyl(2-pentyl-3-oxo-cyclopentyl)acetate 24851-98-7

Sumformula of the chemical	C13H20O3
Water solubility, mg/l	280 (MITI 1992)
Melting point, °C	< -10 (MITI 1992)
Total degradation in water	Biodegradation: 98–99% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

1320 • Methyl acetate 79-20-9

Sumformula of the chemical	C3H6O2
Use	Solvent.
Water solubility, mg/l	245000 20 °C
Boiling point, °C	57
Log octanol/water coefficient, log Pow	0.18 (Sangster 1989)
Volatilization	Relative volatility (nBuAc=1) = 5.10

MNO

LD50 values to mammals in oral exposure, mg/kg	3700	orl-rbt

1321 • Methyl acrylate 96-33-3

Synonyms	Propenoic acid, methyl ester	
Sumformula of the chemical	$C_4H_6O_2$	
Use	Solvent.	
Water solubility, mg/l	49400	20 °C
Boiling point, °C	80	
Log octanol/water coefficient, log Pow	0.8	(Sangster 1989)
Volatilization	Relative volatility (nBuAc=1) = 6.48	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	300	orl-rat
Other information about water organisms	LOEC 64 mg/l, rpd, schr, Uronema parduczi (Bringmann & Kühn 1980b).	

1322 • Methyl benzoate 93-58-3

Synonyms	Benzoic acid, methyl ester Niobe oil	
Sumformula of the chemical	$C_8H_8O_2$	
Use	Perfumery, solvent for cellulose esters and ethers, resins, rubber; flavouring.	
State and appearance	Liquid, colourless, oily.	
Odour	Fragrant odour.	
Specific gravity (water=1)	1.085–1.088	
Boiling point, °C	198.6	
Flashing point, °C	82.7	
Log octanol/water coefficient, log Pow	2.12 2.2	(Anon. 1986) (Sangster 1989)
Other physicochemical properties	Soluble in three parts of 60% alcohol, in most fixed oils, in ether; insoluble in water. Combustible.	

1323 • Methyl biphenyl 28652-72-4

Water solubility, mg/l	< 10	(MITI 1992)
Boiling point, °C	260–270	(MITI 1992)
Total degradation in water	Biodegradation: 41% by BOD (on the upward trend) period: 14d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	

MNO

1324 • Methyl chloroacetate 96-34-4

Sumformula of the chemical	C3H502Cl
EINECS-number	2025011
Water solubility, mg/l	46000 (MITI 1992)
Melting point, °C	< -10 (MITI 1992)
Boiling point, °C	128.5–129.0 (MITI 1992)
Total degradation in water	Biodegradation: 32–75% by BOD (hydrolyzed to methanol and monochloro acetic acid) period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).

1325 • Methyl ether 115-10-6

Synonyms	Dimethyl ether
Sumformula of the chemical	C2H60
Water solubility, mg/l	24000 (MITI 1992)
Melting point, °C	-138.5 (MITI 1992)
Boiling point, °C	-23.6 (MITI 1992)
Log octanol/water coefficient, log Pow	0.1 (Sangster 1989) 0.2 (MITI 1992)
Total degradation in water	Biodegradation: 0–1% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
LC50 values to mammals in inhalation exposure, mg/m³	308000 ihl-rat (Sweet 1987)
LC50 values to mammals in inhalation exposure, ppm	386 ihl-mus, 15 min (Sweet 1987)

1326 • Methyl formate 107-31-3

Synonyms	Methyl methanoate Formic acid, methyl ester
Sumformula of the chemical	C2H402
Use	Solvent.
Molecular weight	60.06
Boiling point, °C	31.5
LD50 values to mammals in oral exposure, mg/kg	1622 orl-rbt (Lewis & Sweet 1984)
LCLo values to mammals in inhalation exposure, ppm	10000 ihl-gpg (Lewis & Sweet 1984)

1327 • Methyl isoamyl ketone

110-12-3

Synonyms	Methylisoamylketone 5-Methyl-2-hexanone
Sumformula of the chemical	C7H14O
Use	Solvent.
Odour	Quality: sweet, sharp Hedonic tone: pleasant Threshold odour concentration absolute: 0.012 ppm 50% recognition: 0.049 ppm 100% recognition: 0.070 ppm Odour index 100% recognition: 75 142 (Hellman & Small 1974)
Boiling point, °C	144
Log octanol/water coefficient, log Pow	1.88 (Sangster 1989)
LD50 values to mammals in oral exposure, mg/kg	4760 orl-rat
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 115 mg/l (Bringmann & Kühn 1980a).
LOEC values to algae, mg/l	90 rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to fishes, mg/l	159 96hr, Pimephales promelas (Veith et al. 1983)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 125 mg/l protozoa (Entosiphon sulcatum): 980 mg/l (Bringmann & Kühn 1980a)

1328 • Methyl isobutyl ketone

108-10-1

Synonyms	4-Methyl-2-pentanone MIBK Isopropylacetone
Use	Solvent.
Odour	Quality: sweet, sharp Hedonic tone: pleasant to unpleasant Threshold odour concentration absolute: 0.10 ppm 50% recognition: 0.28 ppm 100% recognition: 0.28 ppm Odour index 100% recognition: 70 357 (Hellman & Small 1974)
Vapour pressure, mmHg	5 19.7 °C (MITI 1992)
Water solubility, mg/l	20000 20 °C 1.7–2.0% (20 °C) (MITI 1992)
Melting point, °C	-80.26 (MITI 1992)
Boiling point, °C	115.9 (MITI 1992)
Log octanol/water coefficient, log Pow	1.31 (Sangster 1989)

MNO

Volatilization	Relative volatility (nBuAc=1) = 1.60	
Chemical oxygen demand, g 02/g	2.16	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	2.06	5 days (Bridie et al. 1979)
Total degradation in water	Biodegradation: 84% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	2080	orl-rat
LD50 values to birds in oral exposure, mg/kg	> 100	orl-Agelaius phoeniceus (Schafer et al. 1983)
LOEC values to algae, mg/l	136	rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to fishes, mg/l	505	96hr, Pimephales promelas (Veith et al. 1983)
	460	24hr, Carassius auratus (Bridie et al. 1979)
	537	96hr, Pimephales promelas (Broderius & Kahl 1985)

1329 • Methyl methacrylate

80-62-6

Synonyms	2-Methylpropenoic acid, methyl ester	
Sumformula of the chemical	C5H8O2	
Odour	Quality: sweet, sharp Hedonic tone: unpleasant Threshold odour concentration absolute: 0.05 ppm 50% recognition: 0.34 ppm 100% recognition: 0.34 ppm Odour index 100% recognition: 119 705 (Hellman & Small 1974).	
Melting point, °C	-48	(MITI 1992)
Boiling point, °C	100.3	(MITI 1992)
Log octanol/water coefficient, log Pow	1.38	(Sangster 1989)
Total degradation in water	Biodegradation: 94% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LOEC values to algae, mg/l	37	rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
LC50 values to fishes, mg/l	159 232	96hr, Pimephales promelas 96hr, Lepomis macrochirus (Pickering & Henderson 1966)

1330 • 1-Methyl piperidine 626-67-5

Synonyms	N-Methylpiperidine	
Sumformula of the chemical	C6H13N	
Water solubility, mg/l	> 10000	(MITI 1992)
Melting point, °C	-13	(MITI 1992)
Boiling point, °C	106–107	(MITI 1992)
pKa	1.3	(Sangster 1989)
Log octanol/water coefficient, log Pow	1.3 1.36	(Sangster 1989) (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	0.5–1.2 2.6–6.3	6w, Cyprinus carpio, conc 1 mg/l 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	29.8	48hr, Oryzias latipes (MITI 1992)

1331 • 3-Methyl thiophene 616-44-4

Water solubility, mg/l	400	(MITI 1992)
Melting point, °C	13	(MITI 1992)
Boiling point, °C	112.5	(MITI 1992)
Log octanol/water coefficient, log Pow	2.69	(MITI 1992)
Total degradation in water	Biodegradation: 1% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	2.2–6.6 < 3.8	6w, Cyprinus carpio, conc 0.3 mg/l 6w, Cyprinus carpio, conc 0.03 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	20	48hr, Oryzias latipes (MITI 1992)

1332 • 3-Methyl-1-butanol 123-51-3

Synonyms	Isopentanol
Sumformula of the chemical	C5H12O

MNO

Log octanol/water coefficient, log Pow	1.28	(Sangster 1989)
EC50 values to microorganisms, mg/l	4055	Biodegradation inhibition (Vaishnav 1986)

1333 • 2-Methyl-1-pentanol 105-30-6

Synonyms	Amyl methyl alcohol 1,3-Dimethyl alcohol Isohexyl alcohol Isopropyl dimethyl carbinol 2-Methyl-2-propylethanol	
Sumformula of the chemical	C6H14O	
Odour	Quality: sweet, alcohol Hedonic tone: pleasant Threshold odour concentration absolute 0.024 ppm 50% recognition: 0.024 ppm 100% recognition: 0.082 ppm Odour index 100% recognition: 24 024 (Hellman & Small 1974)	
Molecular weight	102.2	
LD50 values to mammals in oral exposure, mg/kg	1410	orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	3560	skn-rbt (Lewis & Sweet 1984)
TCLo values to mammals in inhalation exposure, ppm	50	ihl-hmn (Lewis & Sweet 1984)

1334 • Methyl-2,4-dihydroxybenzoate 2150-47-2

LC50 values to fishes, mg/l	38.5	96hr, Pimephales promelas (Holcombe et al. 1984)

1335 • Methyl-2,5-dichlorobenzoate 2905-69-3

LC50 values to fishes, mg/l	13.8	96hr, Pimephales promelas (Holcombe et al. 1984)

1336 • 6-Methyl-2-aminobenzo-thiazolehydrochloride 2536-91-6

LC50 values to fishes, mg/l	2.2	48hr, Rasbora heteromorpha (Tooby et al. 1975)

1337 • Methyl-2-benzoyl benzoate 606-28-0

Synonyms	2-Benzoyl benzoic acid methyl ester	
Water solubility, mg/l	80	(MITI 1992)
Melting point, °C	52	(MITI 1992)
Boiling point, °C	350–352 (MITI 1992)	

Log octanol/water coefficient, log Pow	2.7	(MITI 1992)
Total degradation in water	Biodegradation: 1% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.3–7.2 < 2.4–14	6w, Cyprinus carpio, conc 0.2 mg/l 6w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	20	48hr, Oryzias latipes (MITI 1992)

1338 • 2-Methyl-2-butanol — 75-85-4

Synonyms	tert-Pentanol	
Sumformula of the chemical	C5H12O	
Log octanol/water coefficient, log Pow	0.89	(Sangster 1989)
LOEC values to algae, mg/l	105	rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
NOEC values to fishes, mg/l	1300	srv, act, Semolitus atromaculatus (Gillette et al. 1952)

1339 • 3-Methyl-2-butanol — 598-75-4

Sumformula of the chemical	C5H12O	
Log octanol/water coefficient, log Pow	1.28	(Sangster 1989)

1340 • 3-Methyl-2-butanone — 563-80-4

Synonyms	Methyl isopropyl ketone	
Sumformula of the chemical	C5H10O	
Use	Solvent.	
Boiling point, °C	93	
Log octanol/water coefficient, log Pow	0.56	(Sangster 1989)
EC50 values to microorganism, mg/l	12404	Biodegradation inhibition (Vaishnav 1986)

1341 • 3-Methyl-2-nitrophenol — 4920-77-8

EC50 values to crustaceans, mg/l	18.8	48hr, mbt, Daphnia magna (Pearson et al. 1979)
LC50 values to fishes, mg/l	46.1	96hr, Pimephales promelas (Pearson et al. 1979)

MNO

1342 • 5-Methyl-2-nitrophenol 700-38-9

Synonyms	6-Nitro-m-cresol	
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 7 mg/l (Bringmann & Kühn 1980a).	
EC50 values to crustaceans, mg/l	21.3	48hr, mbt, Daphnia magna (Pearson et al. 1979)
LC50 values to fishes, mg/l	47	96hr, Pimephales promelas (Pearson et al. 1979)
LOEC values to algae, mg/l	7	rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
Other information about water organisms	LOEC 1.3 mg/l, rpd, schr, Entosiphon sulcatum (Bringmann & Kühn 1980a). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 7 mg/l protozoa (Entosiphon sulcatum): 1.3 mg/l (Bringmann & Kühn 1980a).	

1343 • 4-Methyl-2-pentanol 108-11-2

Synonyms	Isobutylmethylcarbinol Isobutylmethylmethanol Methylamylalcohol	
Sumformula of the chemical	$C_6H_{14}O$	
Use	Solvent.	
Odour	Quality: sweet, alcohol Hedonic tone: unpleasant to pleasant Threshold odour concentration absolute: 0.33 ppm 50% recognition: 0.52 ppm 100% recognition: 0.52 ppm Odour index 100% recognition: 12 634 (Hellman & Small 1974).	
Boiling point, °C	133	
Chemical oxygen demand, g O_2/g	2.6	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g O_2/g	2.82	5 days (Bridie et al. 1979)
LD50 values to mammals in oral exposure, mg/kg	2600	orl-rat
EC50 values to microorganism, mg/l	2452	Biodegradation inhibition (Vaishnav 1986)
LC50 values to fishes, mg/l	360	24hr, Carassius auratus (Bridie et al. 1979)

1344 • n-Methyl-2-pyrrolidone 872-50-4

Use	Solvent.	
Water solubility, mg/l	> 100	(MITI 1992)
Melting point, °C	< -10	(MITI 1992)
Boiling point, °C	210	(MITI 1992)

MNO

Total degradation in water	Biodegradation: 73% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
LD50 values to mammals in oral exposure, mg/kg	7000 orl-rat

1345 • N-Methyl-2-toluidine 611-21-2

Synonyms	2, N-Dimethylaniline N-Methyl-o-toluidine
Sumformula of the chemical	C8H11N
Water solubility, mg/l	> 1000 (MITI 1992)
Boiling point, °C	206–207 (MITI 1992)
pKa	4.6 (Sangster 1989)
Log octanol/water coefficient, log Pow	2.16 (Sangster 1989) 1.95 (MITI 1992)
Total degradation in water	Biodegradation: 1% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	2.7–7.7 6w, Cyprinus carpio, conc 1 mg/l 1.7–8.8 6w, Cyprinus carpio, conc 1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	135 48hr, Oryzias latipes (MITI 1992)

1346 • 2-Methyl-3-(4-tert-butylphenyl)propionaldehyde 80-54-6

Synonyms	p-t-Butyl-α-methylhydro cinnamic aldehyde
Water solubility, mg/l	< 100 (MITI 1992)
Boiling point, °C	105–110, 2 mmHg (MITI 1992)
Total degradation in water	Biodegradation: 8% by BOD (oxized to p-t-Butyl-α- methylhydro cinnamic acid) period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).

MNO

1347 • 5-Methyl-3-heptanone 541-85-5

Synonyms	5-Methylheptan-3-one	
Sumformula of the chemical	C8H16O	
Molecular weight	128.24	
Chemical oxygen demand, g O2/g	1.94	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g O2/g	2.2	5 days (Bridie et al. 1979)
LD50 values to mammals in oral exposure, mg/kg	3500 3800 2500	orl-rat (Lewis & Sweet 1984) orl-mus (Lewis & Sweet 1984) orl-gpg (Lewis & Sweet 1984)
LCLo values to mammals in inhalation exposure, mg/kg	3484 3484	8hr, ihl-rat (Lewis & Sweet 1984) 4hr, ihl-mus (Lewis & Sweet 1984)

1348 • 7-Methyl-3-methylene-1,6-octadiene 123-35-3

Synonyms	1,6-Octadiene, 7-methyl-3-methylene-	
Sumformula of the chemical	C10H16	
EINECS-number	2046225	
Water solubility, mg/l	5.6	(MITI 1992)
Melting point, °C	< -10	(MITI 1992)
Boiling point, °C	93	35 mmHg (MITI 1992)
Log octanol/water coefficient, log Pow	4.17	(MITI 1992)
Total degradation in water	Biodegradation: 82–92% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

MNO

1349 • N-Methyl-3-toluidine 696-44-6

Synonyms	N-Methyl-m-toluidine	
Water solubility, mg/l	1.08	(MITI 1992)
Boiling point, °C	206–207	(MITI 1992)
Log octanol/water coefficient, log Pow	2.19	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

Bioconcentration factor, fishes	5.3–9.9 1.7–7.2	6w, Cyprinus carpio, conc 1 mg/l 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	49.5	48hr, Oryzias latipes (MITI 1992)

1350 • Methyl-4-chlorobenzoate 1126-46-1

LC50 values to fishes, mg/l	10.9	96hr, Pimephales promelas (Holcombe et al. 1984)

1351 • Methyl-4-nitrobenzoate 619-50-1

LC50 values to fishes, mg/l	23.6	96hr, Pimephales promelas (Holcombe et al. 1984)

1352 • Methyl-5-norbornene-2,3-dicarboxylic acid 50853-70-8

Bioconcentration factor, fishes	< 0.5 < 5.5	6w, Cyprinus carpio, conc 1.1 mg/l 6w, Cyprinus carpio, conc 0.11 mg/l (MITI 1992)
LC50 values to fishes, mg/l	359	48hr, Oryzias latipes (MITI 1992)

1353 • Methyl-5-norbornene-2,3-dicarboxylic acid anhydride 25134-21-8

Sumformula of the chemical	C10H1003
Total degradation in water	Biodegradation: 0% byb BOD (hydrolyzed to Methyl-5-norbornene-2,3-dicarboxylic acid) period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

1354 • N-Methyl-N-oleoyltaurine sodium salt 137-20-2

Sumformula of the chemical	C21H4004NNa
Total degradation in water	Biodegradation: 75% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

1355 • 3-Methylacetanilide 537-92-8

Synonyms	N-(3-Methylphenyl)ethanamide
Sumformula of the chemical	C9H11NO

MNO

Log octanol/water coefficient, log Pow	1.59	(Sangster 1989)
Log soil sorption coefficient, log Kom	1.21	(Sabljic 1987)

1356 • N-Methylacetanilide 579-10-2

Water solubility, mg/l	16.7	(MITI 1992)
Melting point, °C	102–104	(MITI 1992)
Boiling point, °C	253	(MITI 1992)
Log octanol/water coefficient, log Pow	1.29	(MITI 1992)
Total degradation in water	Biodegradation: 1% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	0.37–0.74 < 1.7	6w, Cyprinus carpio, conc 1 mg/l 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	364	48hr, Oryzias latipes (MITI 1992)

1357 • 4-Methylacetophenone 122-00-9

Sumformula of the chemical	C9H10O	
Log octanol/water coefficient, log Pow	2.19	(Sangster 1989)

1358 • 2-(Methylamino)benzoic acid 119-68-6

Synonyms	2-(N-Methylamino)benzoic acid	
Water solubility, mg/l	> 100	(MITI 1992)
Melting point, °C	182	(MITI 1992)
Total degradation in water	Biodegradation: 85% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	

1359 • 4-(Methylamino)benzoic acid 10541-83-0

Synonyms	p-(Methylamino)benzoic acid	
Water solubility, mg/l	1.2	(MITI 1992)

Melting point, °C	168	(MITI 1992)
Log octanol/water coefficient, log Pow	1.01	(MITI 1992)
Total degradation in water	Biodegradation: 14% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.2–0.3 < 2.4	6w, Cyprinus carpio, conc 0.5 mg/l 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	220	48hr, Oryzias latipes (MITI 1992)

1360 • p-Methylaminophenol 150-75-4

LC50 values to fishes, mg/l	0.5	48hr, Carassius auratus (McKee & Wolf 1963)
	0.3	act, Salmo gairdneri (Hodson et al. 1984)

1361 • 4-Methylaminophenolsulfate 55-55-0

Synonyms	p-Hydroxymethylaniline	
Use	Reducing agent used primarily in the development of silver sensitized films and papers.	
Molecular weight	219.23	
Melting point, °C	260	dec.
LDLo values to mammals in oral exposure, mg/kg	200	orl-rat (Lewis & Sweet 1984)
NOEC values to algae, mg/l	10	rpd, schr, Selenastrum capricornutum (Verschueren 1983)
LC50 values to crustaceans, mg/l	0.019	Daphnia magna (Verschueren 1983)
LC50 values to fishes, mg/l	0.25	act, Pimephales promelas (Verschueren 1983)

1362 • 2-Methylaniline 95-53-4

Synonyms	o-Amino-toluene 2-Amino-1-methylbenzene o-Toluidine o-Methyl aniline	
Sumformula of the chemical	C7H9N	
Use	Intermediate.	
State and appearance	Colourless liquid.	
Molecular weight	107.17	
Vapour pressure, mmHg	0.1	20 °C
Water solubility, mg/l	15000	25 °C

MNO

Boiling point, °C	200–202 (MITI 1992)
pKa	4.43 (Sangster 1989)
Log octanol/water coefficient, log Pow	1.3 Anon. 1988 1.32 (Sangster 1989)
Henry's law constant, Pa x m^3/mol	0.093 (Anon. 1988)
Mobility	Equilibrium distribution: *mass %* air 3.10 water 96.61 solid 0.29 (Anon. 1988).
Total degradation in soil	Biodegradation: decomposition by a soil micro flora in > 64 days (Verschueren 1983).
Total degradation in water	Biodegradation: 65.4% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
Other information about degradation	Degradation by Aerobacter (500 mg/l, 30 °C): parent: 100% ring disruption in 64 hours mutant: 100% ring disruption in 6 hours (Verschueren 1983).
LD50 values to mammals in oral exposure, mg/kg	670 orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	3250 skn-rbt (Lewis & Sweet 1984)
LDLo values to mammals in oral exposure, mg/kg	300 orl-cat 5 orl-frg (Lewis & Sweet 1984)
TCLo values to mammals in inhalation exposure, mg/kg	25 ihl-man (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	100–316 orl-Agelaius phoeniceus 100–422 orl-Sturnus vulgaris ≥ 1000 orl-Coturnix coturnix 750 orl-Passer domesticus (Schafer et al. 1983)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 16 mg/l (Bringmann & Kühn 1980a).
LOEC values to algae, mg/l	0.31 rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976) 6.3 rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
Other information about water organisms	EC50 (24hr) 520 mg/l, rpd, Tetrahymena pyriformis (Yoshioka et al. 1985). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 6.3 mg/l protozoa (Entosiphon sulcatum): 76 mg/l (Bringmann & Kühn 1980a).

1363 • 3-Methylaniline 108-44-1

Synonyms	3-Toluidine m-Toluidine	
Sumformula of the chemical	C7H9N	
Water solubility, mg/l	10	(MITI 1992)
Melting point, °C	-31.2	(MITI 1992)
Boiling point, °C	203.3	(MITI 1992)
Log octanol/water coefficient, log Pow	1.4 1.53	(Sangster 1989) (MITI 1992)
Log soil sorption coefficient, log Kom	1.41	(Sabljic 1987)
Total degradation in water	Biodegradation: 0–1% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
LD50 values to birds in oral exposure, mg/kg	242 > 1000 562	orl-Agelaius phoeniceus orl-Sturnus vulgaris orl-Coturnix coturnix (Schafer et al. 1983)
LC50 values to crustaceans, mg/l	0.73	48hr, Daphnia magna (Hermens et al. 1984)
EC50 values to crustaceans, mg/l	0.043	rpd, 16d, Daphnia magna (Hermens et al. 1984)

1364 • 4-Methylaniline 106-49-0

Synonyms	p-Toluidine	
Sumformula of the chemical	C7H9N	
pKa	5.08	(Sangster 1989)
Log octanol/water coefficient, log Pow	1.39	(Sangster 1989)
Log soil sorption coefficient, log Kom	1.66	(Sabljic 1987)
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LD50 values to birds in oral exposure, mg/kg	56.2 42.2 237 237	orl-Agelaius phoeniceus orl-Sturnus vulgaris orl-Coturnix coturnix orl-Passer domesticus (Schafer et al. 1983)

1365 • N-Methylaniline 100-61-8

Sumformula of the chemical	C7H9N
Use	Intermediate.
Molecular weight	107

MNO

Melting point, °C	-57	(MITI 1992)
Boiling point, °C	195.7	(MITI 1992)
pKa	4.85	(Sangster 1989)
Log octanol/water coefficient, log Pow	1.7 1.66	(Anon. 1988) (Sangster 1989)
Henry's law constant, Pa x m³/mol	0.27	(Anon. 1988)
Mobility	Equilibrium distribution: air water solid	 *mass %* 8.41 90.89 0.70 (Anon. 1988).
Total degradation in water	Biodegradation: 1.4% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).	
Bioconcentration factor, fishes	0.7–4.1 < 10	6w, Cyprinus carpio, conc 1 mg/l 6w, Cyprinus carpio, conc 0.1mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	98	48hr, Oryzias latipes (MITI 1992)

1366 • 9-Methylanthracene 779-02-2

Sumformula of the chemical	C15H12	
Log octanol/water coefficient, log Pow	5.07 5.07	(Mackay 1982) (Sangster 1989)
Effects on arthropods	LC50, 1 d: 0.0064 mg/l, Aedes aegypti; 0.270 mg/l, Aedes taeniorhynchus; 0.037 mg/l, Culex quinquefasciatus (Borovsky et al. 1987).	

1367 • Methylazoxymethanol acetate 592-62-1

Effects on the physiology of water organisms	Poecilia reticulata, 2 mg/l, 0.08 d, histological effect (presence of physical damage to tissues) (Fournie et al. 1987).

1368 • 2-Methylbenzoic acid 118-90-1

Sumformula of the chemical	C8H8O2	
Water solubility, mg/l	> 900	(MITI 1992)
Melting point, °C	102–105	(MITI 1992)

MNO

pKa	3.92	(Sangster 1989)
Log octanol/water coefficient, log Pow	2.46	(Sangster 1989)
Total degradation in water	Biodegradation: 91–96% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	

1369 • 3-Methylbenzoic acid 99-04-7

Synonyms	m-Toluic acid	
Sumformula of the chemical	C8H8O2	
Use	Organic synthesis, to form N, N-diethyl-m-toluamide, a broad-spectrum insect repellent.	
State and appearance	White to yellowish crystals.	
Specific gravity (water=1)	1.0543	
Melting point, °C	109	
Boiling point, °C	263	
pKa	4.27	(Sangster 1989)
Log octanol/water coefficient, log Pow	2.37 2.37	(Anon. 1986) (Sangster 1989)
Other physicochemical properties	Slightly soluble in water, soluble in alcohol and ether. Combustible.	

1370 • 4-Methylbenzoic acid 99-94-5

Sumformula of the chemical	C8H8O2	
pKa	4.39	(Sangster 1989)
Log octanol/water coefficient, log Pow	2.34	(Sangster 1989)

1371 • 4-Methylbenzyl alcohol 589-18-4

Sumformula of the chemical	C8H10O	
Log octanol/water coefficient, log Pow	1.6 1.58	(Anon. 1986) (Sangster 1989)

1372 • α-Methylbenzylamine 89-93-0

Sumformula of the chemical	C8H11N	
EINECS-number	2019521	
Boiling point, °C	187.5	(MITI 1992)

MNO

Log octanol/water coefficient, log Pow	0.863 (MITI 1992)
Total degradation in water	Biodegradation: 6% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).
Bioconcentration factor, fishes	1.0–2.9, 6w, Cyprinus carpio, conc 0.5 mg/l < 2.6–6.6 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
LC50 values to fishes, mg/l	48 48hr, Oryzias latipes (MITI 1992)

1373 • Methylbromide 74-83-9

Synonyms	Bromomethane Zytox Profume Rotox Bromosol Brozone Monobromomethane Dowfume
Sumformula of the chemical	CH3Br
Purity, %	99.5
Use	Ionization chambers; decreasing wool; extracting oils; fumigant; refrigerant; fire extinguishing agents.
State and appearance	Colourless gas. Will cling close to ground but will not dissolve to any great extent. Also available as a liquefied gas.
Molecular weight	94.94
Specific gravity (water=1)	1.737 at -10 °C
Vapour density (air=1)	3.27
Vapour pressure, mmHg	1250 20 °C 1140.8 15.6 °C (MITI 1992)
Water solubility, mg/l	18000 (MITI 1992)
Melting point, °C	-93.7 (MITI 1992)
Boiling point, °C	3.56 (MITI 1992)
Log octanol/water coefficient, log Pow	1.19 (Sangster 1989) 1.08 (MITI 1992)
Henry's law constant, Pa x m³/mol	687.4 calc. (Yaws et al. 1991)
Total degradation in water	Biodegradation: 17% by BOD period: 28d substance 5.01 mg/l sludge 2 mg/l 15% by BOD period 28d substance 10.0 mg/l sludge 2 mg/l (MITI 1992).

Other information about degradation	Will volatilize off rapidly. Does not persist in sunlight. Photodissociation not significant until it reaches the stratosphere. Hydrolysis half-life at 25 °C and pH 7 of 20 days, so is probably as important removal mechanism, after volatilization (Sax 1986).	
Other information about bioaccumulation	Initial rapid elimination through lungs as bromomethane and urine as bromide, final elimination takes longer, accounting in part for prolonged toxicity. Log octanol/water partition coefficient – 1.1 so probably does not have significant tendency to bioaccumulate (Sax 1986).	
LD50 values to mammals in oral exposure, mg/kg	214	orl-rat (Sweet 1987)
LC50 values to mammals in inhalation exposure, mg/m³	1540	ihl-mus, 2hr (Sweet 1987)
LC50 values to mammals in inhalation exposure, ppm	302	ihl-rat, 8hr (Sweet 1987)
LCLo values to mammals in inhalation exposure, mg/kg	1000 2000	2hr, ihl-child 11hr, ihl-rbt (Sax 1986)
LCLo values to mammals in inhalation exposure, ppm	2000 300 60000 3120	ihl-rat 9hr, ihl-gpg 2hr, ihl-man 15min, ihl-rat ihl-rat 9hr, ihl-gpg 2hr, ihl-man 15min, ihl-rat ihl-rat 9hr, ihl-gpg 2hr, ihl-man 15min, ihl-rat ihl-rat 9hr, ihl-gpg 2hr, ihl-man 15min, ihl-rat (Sax 1986)
TDLo values to mammals in oral exposure, mg/kg	3250	orl-rat, tumorigenic (Sweet 1987)
TCLo values to mammals in inhalation exposure, ppm	35	ihl-hmn (Sax 1986)
Other information about mammals	Toxic: 150 mg/kg, orl-dog, in food (Sax 1986). Limb paralysis, other toxic effects: 20–120 mg/kg, scu-rbt, in oil (Sax 1986).	
Health effects	Strong irritant. Direct skin contact-prickling, itching, cold sensation, erythemia (redness), vesication (blister), burns, damage to peripheral nerve tissue, delayed dermatitis. Eye irritation (Sax 1986). Double vision, nausea, dizziness, headache. Severe exposure, convulsions, muscular tremors, possibly death. Can cause fatal pulmonary edema. Levels of 100–500 ppm can cause nonfatal poisoning. May leave permanent injury. Can be absorbed via skin. Neurological and gastrointestinal disturbances. In severe cases, there is a latent period up to 48 hours before symptoms occur, and recovery can be quite long with persisting neurological disorders (Sax 1986). Highly toxic when ingested or inhaled. Moderately toxic via all routes with chronic exposure. Emits highly toxic vapours when heated to decomposition. Has mutagenic potential. Has latent period and its presence is difficult to detect, so prolonged and more severe exposure may occur (Sax 1986).	

Mutagenicity	Affects DNA causing point mutations and large chromosome alterations. Positive in one strain of Salmonella typhimurium without activation, when tested as a gas (Sax 1986). mmo, sat 400 ppm (Sax 1986). Mutation data: gene mutation in mammalian cells: mus, lym, 0.3 mg/l; microbial mutation without S9: klp, 4750 mg/m³; sat, 400ppm; mma, sat 5000 mg/m³; sin, dmg, ihl, 150 mg/m³, 6hr; sce, hmn, lym, 43000 ppm (Sweet 1987).	
LC50 values to fishes, mg/l	11 12	96hr, Lepomis macrochirus 96hr, Menidia audens (Dawson et al. 1977)

1374 • 3-Methylbutanal

590-86-3

Synonyms	Isovaleraldehyde Isoamylaldehyde	
Sumformula of the chemical	C5H10O	
Purity, %	> 99%	
Known impurities	Major impurity: 3-methyl butanol	
Use	Only used as intermediate. Industrial use in closed system. No public use Export (BASF AG)	
Water solubility, mg/l	20000	at 20 °C (BASF AG)
Boiling point, °C	91–93 °C	101.3 kPa, DIN 51751 (BASF AG)
Solidification point, °C	-51	BS 523/1964 (BASF AG)
Flashing point, °C	0	closed cup, DIN 51755 (BASF AG)
Log octanol/water coefficient, log Pow	1.31	at 25 °C, measured, OECD No. 107 (BASF AGa)
Other information about degradation	BOD5 x 100/COD > 60%, aerobic, DIN 38409 L 51 (BOD5) DIN 38409 L 43 (COD) Readily biodegradable (BASF AG)	
LD50 values to mammals in oral exposure, mg/kg	6200	about 6200, orl-rat (BASF AGb)
LD50 values to mammals in non-oral exposure, mg/kg	2730	skn-rbt (Carpenter et al. 1974)
Effects on microorganisms	EC0 = 310.0 mg/l, DIN 38412 L8, Pseudomonas putida (BASF AGc 1988, 330168/1988)	
EC50 values to algae, mg/l	80	72hr, DIN 38412 L9, Scenedesmus subspicatus (BASF AGc 1988)
EC50 values to crustaceans, mg/l	176.8	48hr, EC Directive 79/831 EEC Annex V C.2, Daphnia magna Strauss (BASF AGc 1988 (1023/88))
LC50 values to fishes, mg/l	3.3 53 13.3	96hr, Pimephales promelas (Geiger et al. 1989) 96hr, Leuciscus idus (BASF AGb 1989, 10F0712/885067, 28.06.89) 2w, Lebistes reticulatus (Deneer et al. 1988)
Other information	Isovaleraldehyde is readily biodegradable and shows a low potential for bioaccumulation and low acute toxic effects against Daphnia; therefore no long-term testsare required. (BASF AG).	

MNO

1375 • Methylchloride 74-87-3

Synonyms	Chloromethane	
Sumformula of the chemical	CH3Cl	
Use	Solvent.	
Vapour pressure, mmHg	3671.9	20 °C (MITI 1992)
Water solubility, mg/l	7500 7300	20 °C 20 °C (MITI 1992)
Melting point, °C	-97.72	(MITI 1992)
Boiling point, °C	-23.76	(MITI 1992)
Log octanol/water coefficient, log Pow	0.91 0.85	(Sangster 1989) (MITI 1992)
Henry's law constant, Pa x m³/mol	836.8	calc. (Yaws et al. 1991)
Total degradation in water	Biodegradation: 1% by BOD period: 28d substance: 3.79 mg/l sludge: 2 mg/l 0% by BOD period: 28d substance: 19.2 mg/l sludge 2 mg/l (MITI 1992).	
LCLo values to mammals in inhalation exposure, ppm	3146	ihl-mus
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 500 mg/l (Bringmann & Kühn 1980a)	
LOEC values to algae, mg/l	550	rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to fishes, mg/l	550 270	96hr, Lepomis macrochirus 96hr, Menidia audens (Dawson et al. 1977)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 1450 mg/l protozoa (Entosiphon sulcatum): > 8000 mg/l (Bringmann & Kühn 1980a)	

1376 • 3-Methylcholanthrene 56-49-5

Sumformula of the chemical	C21H16	
Log octanol/water coefficient, log Pow	6.75	(Sangster 1989)
Log soil sorption coefficient, log Kom	6.25 6.13	observed (Sabljic 1987) calculated (Sabljic 1987)
Effects on the physiology of water organisms	10 mg/kg, 2 d, changes in the RNA and DNA of the cell: Ctenopharyngodon idella, Cyprinus carpio, Tinca tinca (Al-Sabti 1986). Salmo gairdneri, 80 mg/kg, 6 d, biochemical effect (change in physicochemical process including glycogen uptake, cholesterol levels and lipid analysis) (Miyauchi & Uematsu 1987).	

MNO

1377 • Methylcyclohexane 108-87-2

Sumformula of the chemical	C7H14	
EINECS-number	2036243	
Water solubility, mg/l	22	(MITI 1992)
Melting point, °C	-126.6	(MITI 1992)
Boiling point, °C	100.9	(MITI 1992)
Henry's law constant, Pa x m^3/mol	43280	calc. (Yaws et al. 1991)
Log octanol/water coefficient, log Pow	4.13 3.88	(MITI 1992) (Sangster 1989)
Total degradation in water	Biodegradation: 0% by BOD (closed bottle test) period: 28d substance: 10 mg/l sludge: 2 mg/l (MITI 1992).	
Bioconcentration factor, fishes	95–321 134–237	8w, Cyprinus carpio, conc 0.1 mg/l 8w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LDLo values to mammals in oral exposure, mg/kg	4000	orl-rbt
LC50 values to fishes, mg/l	5.02 0.24	48hr, Oryzias latipes (MITI 1992) 96hr, Leuciscus idus (Hartwell 1951)
Other information	Less toxic as emulsion (LC50(96hr), 72 mg/l (Hartwell 1951)).	

MNO

1378 • 4-Methylcyclohexane-1,2-dicarboxylic acid 57567-84-7

Sumformula of the chemical	C9H14O4	
Bioconcentration factor, fishes	< 0.2 < 2.4	6w, Cyprinus carpio, conc 0.5 mg 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 500	48hr, Oryzias latipes (MITI 1992)

1379 • 4-Methylcyclohexane-1,2-dicarboxylic anhydride 19438-60-9

Synonyms	4-Methylcyclohexane-1,2-dicarboxylic acid anhydride
Water solubility, mg/l	> 1000 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD (hydrolyzed to 4-methylcyclohexane-1,2-dicarboxylic acid) period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).

1380 • 2-Methylcyclohexanone 583-60-8

Use	Solvent.	
Boiling point, °C	173	
LD50 values to mammals in oral exposure, mg/kg	2140	orl-rat
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 60 mg/l (Bringmann & Kühn 1980a)	
LOEC values to algae, mg/l	88	rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
	26	rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 88 mg/l protozoa (Entosiphon sulcatum): 160 mg/l (Bringmann & Kühn 1980a)	

1381 • 4,4'-Methylene bis(2,6-di-t-butylphenol) 118-82-1

Synonyms	Phenol, 4,4'-methylenebis(2,6-bis(1,1-dimethylethyl)-	
Sumformula of the chemical	C29H4402	
EINECS-number	2042791	
Bioconcentration factor, fishes	3.4–13.4 14–64.5	6w, Cyprinus carpio, conc 1 mg/l 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
LC50 values to fishes, mg/l	160	48hr, Oryzias latipes (MITI 1992)

1382 • Methylene blue 61-73-4

LC50 values to crustaceans, mg/l	100	96hr, Penaeus californiensis (Hanks 1976)

1383 • 2,2'-Methylenebis(6-t-buthyl-4-methylphenol 119-47-1

Synonyms	Phenol, 2,2'-methylenebis(6-(1,1-dimethylethyl)-4-methyl-	
Sumformula of the chemical	C23H3202	
EINECS-number	2043271	
Water solubility, mg/l	0.02	(MITI 1992)
Melting point, °C	126.5–130	(MITI 1992)
Log octanol/water coefficient, log Pow	6.25	(MITI 1992)

MNO

Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	23–37 60–125	8w, Cyprinus carpio, conc 0.001 mg/l 8w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 500	48hr, Oryzias latipes (MITI 1992)

1384 • Methylenebisthiocyanate 6317-18-6

Use	Slimicide.	
LOEC values to fishes, mg/l	1.5–2.0	srv, juv. Branchydanio rerio (Björndal et al. 1984)

1385 • 2-Methylfuran 534-22-5

LD50 values to birds in oral exposure, mg/kg	> 98	Agelaius phoeniceus (Schafer et al. 1983)
LOEC values to algae, mg/l	40	rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
	40	rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
Other information about water organisms	LOEC 26 mg/l, rpd, schr, Uronema parduczi (Bringmann & Kühn 1976).	

1386 • 2-Methyllactonitrile 75-86-5

Synonyms	α-Hydroxyisobutyronitrile Acetone cyanohydrin 2-Hydroxy-2-methylpropionitrile 2-Hydroxy-2-methylpropanenitrile	
Sumformula of the chemical	C4H7NO	
Use	Insecticides; intermediate for organic synthesis especially methylmethacrylate.	
State and appearance	Colourless liquid.	
Molecular weight	85.12	
Specific gravity (water=1)	0.93	19 °C
Vapour density (air=1)	2.95	
Conversion factor, 1 ppm in air=	3.54	mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.28	ppm
Vapour pressure, mmHg	0.8	at 20 °C
Water solubility, mg/l	> 100000	(MITI 1992)
Melting point, °C	-19	(MITI 1992)
Boiling point, °C	82	(MITI 1992)
Degradation point, °C	120	

MNO

Total degradation in water	Biodegradation: 95% by GC analysis period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	15 9 14 17.8 13.5	orl-mus (Verschueren 1983) orl-gpg orl-mus orl-rat orl-rbt (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	1	ipr-mus (Sweet 1987)
LDLo values to mammals in non-oral exposure, mg/kg	8.5 150 17	scu-rat skn-gpg skn-rbt (Sweet 1987)
LCLo values to mammals in inhalation exposure, mg/kg	500	ihl-mus, 2hr (Sweet 1987)
LCLo values to mammals in inhalation exposure, ppm	63	ihl-rat (Sweet 1987)

1387 • Methylmercaptan

74-93-1

Synonyms	Methanethiol Methylthioalcohol	
State and appearance	Colourless gas.	
Molecular weight	48.11	
Melting point, °C	-123.1	
Boiling point, °C	6–7.6	
LC50 values to mammals in inhalation exposure, mg/m³	1700	2hr, ihl-mus (Lewis & Sweet 1984)
LC50 values to mammals in inhalation exposure, ppm	675	1.35 mg/l, ihl-rat (Lewis & Sweet 1984)
LC50 values to fishes, mg/l	0.95 0.65	96hr, Oncorhynchus kisutch 120hr, Oncorhynchus tshawytscha (Adelman & Smith Jr. 1972)

1388 • Methylmercuric chloride

115-09-3

Sumformula of the chemical	CH3HgCl
Mobility	Transformation to methylmercury is the most important part of Hg cycle in the environment. Hg is strongly bound to organic matter is soil and sediment. – Inorganic Hg compounds are methylized abiotically in the presence of methylcobalamine (B12-CH3) and biotically with help of enzymes (Hg2+ → CH3Hg+ + / (CH3)2Hg) (Kaiser & Tölg 1980).

MNO

Other information about degradation	Organic Hg compounds kan be formed and break up chemically, biochemically and through photosynthesis as well in atmosphere as in aquatic environment: $CH_3Hg^+ \leftrightarrow (CH_3)_2Hg \leftrightarrow Hg \leftrightarrow Hg^{2+}$ (Anon. 1989).
Metabolism in mammals	Inorganic Hg is mainly stored in kidneys (WHO 1976). Organic Hg compounds decompose to inorganic Hg and accumulates in kidneys (WHO 1976). Methylmercury is absorbed in alimentary canal 90–100% after intake with food, whereas inorganic Hg is absorbed less than 15% (WHO 1976). Brains seem to be very sensitive to methylmercury and for Hg vapour (Berlin 1986). Methylmercury is very slowly decombosed mainly through faeces (Berlin 1986).
LD50 values to mammals in non-oral exposure, mg/kg	14–17 ipr-mus (Laveskog et al. 1976)
Health effects	Inorganic bivalent Hg compounds and unstabile organic Hg compounds induce damages in kidneys (Berlin 1986). Methylmercury has effects on the central nervous system – motoric and mental disorders etc. (Berlin 1986).
LOEC values to crustaceans, mg/l	0.002 Artemia salina (Cunningham & Grosch 1978)
LC50 values to fishes, mg/l	0.08 24hr, Carassius auratus (Sharma & Davis 1980) 0.024-0.042 96hr, Salmo gairdneri (Perwak et al. 1985)
Effects on the physiology of water organisms	Lepomis macrochirus, 0.0000000000034 M, 1 d, change in enzyme activity (Baatrup & Danscher 1987).
Other effects on aquatic ecosystems	Phytoplankton, marine, 0.0005 mg/l (Knauer & Martin 1972). Salvelinus fontinalis, grw, 16 + 21 days, 0.0009 (Christensen 1975). Salmo gaidneri, sperm, srv, 30 min, > 1 mg/l (McIntyre 1973). Lepomis, enzymes, 0.0000000085 mg/l (Hossain & Dutta 1983).

1389 • Methylmercury 22967-92-6

Sumformula of the chemical	CH_3Hg
Molecular weight	215.63
Mobility	Transformation to methylmercury is the most important part of Hg cycle in the environment. Hg is strongly bound to organic matter is soil and sediment. – Inorganic Hg compounds are methylized abiotically in the presence of methylcobalamine (B12-CH3) and biotically with help of enzymes ($Hg^{2+} \rightarrow CH_3Hg^+$ + / $(CH_3)_2Hg$) (Kaiser & Tölg 1980).
Other information about degradation	Organic Hg compounds can be formed and break up chemically, biochemically and through photosynthesis as well in atmosphere as in aquatic environment: $CH_3Hg^+ \leftrightarrow (CH_3)_2Hg \leftrightarrow Hg \leftrightarrow Hg^{2+}$ (Anon. 1989).
Metabolism in mammals	Inorganic Hg is mainly stored in kidneys (WHO 1976). Organic Hg compounds decompose to inorganic Hg and accumulates in kidneys (WHO 1976). Methylmercury is absorbed in alimentary canal 90–100% after intake with food, whereas inorganic Hg is absorbed less than 15% (WHO 1976). Brains seem to be very sensitive to methylmercury and for Hg vapour (Berlin 1986). Methylmercury is very slowly decomposed mainly through faeces (Berlin 1986).
Bioconcentration factor, fishes	100000 pike (Monitor 1987)

Other information about bioaccumulation	Half-life, fish, 1000 days (Monitor 1987).	
Health effects	Inorganic bivalent Hg compounds and unstable organic Hg compounds induce damages in kidneys (Berlin 1986). Methylmercury has effects on the central nervous system – motoric and mental disorders etc. (Berlin 1986).	
LOEC values to crustaceans, mg/l	0.002	Artemia salina, rpd, schr (Cunningham & Grosch 1978)
LC50 values to fishes, mg/l	0.089	96hr, Trichogaster trichopterus (Roales & Perlmutter 1974)
LOEC values to fishes, mg/l	0.00013	rpd, srv, chr, Pimephales promelas (McKim 1977)
	0.0009	srv, chr, Salvelinus fontinalis (McKim et al. 1977)
	0.00033	rpd, grw, chr, flagfish (McKim 1977)
NOEC values to fishes, mg/l	0.00007	rpd, srv, chr, Pimephales promelas (McKim 1977)
	0.0003	srv, chr, Salvelinus fontinalis (McKim et al. 1977)
	0.00017	rpd, grw, chr, flagfish (McKim 1977)

1390 • 1-Methylnaphthalene 90-12-0

Henry's law constant, Pa x m³/mol	36.48	calc. (Yaws et al. 1991)
LC50 values to fishes, mg/l	9	96hr, Pimephales promelas (Vincent et al. 1976)
	8.4	48hr, Salmo trutta m. lacustris (Woodiwiss & Fretwell 1974)

1391 • Methylparathion 298-00-0

Synonyms	0,0-Dimethyl-0-4-nitrophenylphosphorothioate	
Use	Insecticide.	
Molecular weight	263.22	
Water solubility, mg/l	55–60	
Half-life in soil, days	15	(Li et al. 1990)
Total degradation in water	0% original compound found after 4 weeks in river water (initial concentration 10 µg/l) (Verschueren 1983).	
LD50 values to mammals in oral exposure, mg/kg	6 23	orl-rat orl-mus (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	63	skn-rat (Lewis & Sweet 1984)
Carcinogenicity	NCI carcinogenesis bioassay completed: results negative; mus, rat (Lewis & Sweet 1984).	
LD50 values to birds in oral exposure, mg/kg	7	orl-bwd (Lewis & Sweet 1984)
	10 7.5	orl-Agelaius phoeniceus orl-Sturnus vulgaris (Schafer et al. 1983)
LD50 values to birds in dermal exposure, mg/kg	54	skn-dck (Lewis & Sweet 1984)

MNO

LC50 values to crustaceans, mg/l	0.0048	Daphnia pulex (Frear & Boyd 1967)
	0.0008	96hr, Mysidopsis bahia
	0.0012	96hr, Penaeus duorarum (Anon. 1981) (EPA 600/4-81-041)
	0.009	act, Daphnia pulex (Nishiuchi & Hashimoto 1967)
	0.005	act, Daphnia magna (Kenaga 1979)
	0.89	96hr, Acartia tonsa (Khattat & Farley 1976)
	0.002	96hr, Crangon septemspinosa (Macek & McAllister 1970)
LC50 values to fishes, mg/l	2.7	96hr, Salmo gairdneri (Pesticide Manual 1983)
	0.059	96hr, Leistomus canthurus (Anon. 1981) (EPA 600/4-81-041)
	6.34–11	96hr, Labeo rohita (Bengeri et al. 1984)
	2.8	96hr, Salmo gaidneri (Palawski et al. 1983)
	0.26	48hr, Sarotheredon (Rao & Rao 1982)
	7	96hr, Heteropneustes fossilis (Singh & Srivastava 1982)
	5.4–6.9	96hr, Pimephales promelas (Järvinen & Tanner 1982)
	12	48hr, Cyprinus carpio (Nagaratnamma & Ramamurthi 1981)
	7.5	48hr, Cyprinus carpiourus (Nishiuchi & Hashimoto 1967)
	5.72	act, Lepomis macrochirus
	2.75	act, Salmo gairdneri
	8.9	act, Pimephales promelas (Kenaga 1979)
	2.75	96hr, Salmo gairdneri
	4.74	96hr, Salmo trutta m. lacustris
	3.06	96hr, Perca flavescens (Macek & McAllister 1970)
	2.7	24hr, Salmo gairdneri (Edwards 1977)
LOEC values to fishes, mg/l	0.59	grw, schr, Pimepales promelas (Järvinen & Tanner 1982)
NOEC values to fishes, mg/l	0.31	grw, schr, Pimepales promelas (Järvinen & Tanner 1982)
Other information about water organisms	LOEC 6.3 mg/l, Colpidium campylum (Dive et al. 1980).	

MNO

1392 • 1-Methylphenanthrene 832-69-9

Sumformula of the chemical	C15H12	
Log octanol/water coefficient, log Pow	5.08	(Sangster 1989)

1393 • 2-Methylpropanal 78-84-2

Synonyms	Isobutyraldehyde
Odour	Quality: sweet, ester Hedonic tone: pleasant to unpleasant Threshold odour concentration absolute: 0.047 ppm 50% recognition: 0.141 ppm 100% recognition: 0.236 ppm Odour index 100% recognition: 766 949 (Hellman & Small 1974).

Water solubility, mg/l	300	(MITI 1992)
Melting point, °C	-66	(MITI 1992)
Boiling point, °C	63–64	(MITI 1992)
Total degradation in water	Biodegradation: 81% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	

1394 • 2-Methylpropenoic acid, ethyl ester 97-63-2

Sumformula of the chemical	C6H10O2	
Log octanol/water coefficient, log Pow	1.94	(Sangster 1989)

1395 • 2-Methylpropenoic acid, isopropyl ester 4655-34-9

Sumformula of the chemical	C7H12O2	
Log octanol/water coefficient, log Pow	2.25	(Sangster 1989)

1396 • 2-Methylpropenoic acid, n-butyl ester 97-88-1

Sumformula of the chemical	C8H14O2	
Log octanol/water coefficient, log Pow	2.88	(Sangster 1989)

1397 • Methylpropionate 554-12-1

Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 330 mg/l (Bringmann & Kühn 1980a).	
LOEC values to algae, mg/l	11	rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
	13	rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 11 mg/l protozoa (Entosiphon sulcatum): 311 mg/l (Bringmann & Kühn 1980a).	

1398 • 2-Methylpropyl amine 78-81-9

Synonyms	1-Amino-2-methylpropane Isobutylamine	
Sumformula of the chemical	C4H11N	
Melting point, °C	-84.6	(MITI 1992)

MNO

Boiling point, °C	68.9 (MITI 1992)
pKa	10.56 (Sangster 1989)
Log octanol/water coefficient, log Pow	0.73 (Sangster 1989)
Total degradation in water	Biodegradation: 87% (NH3) by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l 68% (NO2) by BOD period: 14d substance: 100 mg/l sludge 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

1399 • 4-(1-Methylpropyl)phenol 99-71-8

Synonyms	p-sec-Butylphenol
Water solubility, mg/l	> 100 (MITI 1992)
Melting point, °C	60 (MITI 1992)
Log octanol/water coefficient, log Pow	1.4 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	0.93–30 6w, Cyprinus carpio, conc 0.02 mg/l < 3.7–37 6w, Cyprinus carpio, conc 0.002 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	2.9 48hr, Oryzias latipes (MITI 1992)

1400 • Methylpyridine 108-89-4

Synonyms	γ-Picoline
pKa	6.02 (Sangster 1989)
Log octanol/water coefficient, log Pow	1.22 (Sangster 1989)
LD50 values to birds in oral exposure, mg/kg	100–1000 orl-Agelaius phoeniceus > 1000 orl-Sturnus vulgaris 422 orl-Coturnix coturnix 1000 orl-Passer domesticus (Schafer et al. 1983)
Other information about water organisms	EC50 (60hr), 730 mg/l, rpd, Tetrahymena pyriformis (Schultz & Mouton 1985).

MNO

1401 • 2-Methylpyridine 109-06-8

Synonyms	2-Picoline
Sumformula of the chemical	C6H7N
Odour	Quality: sweet Hedonic tone: unpleasant Threshold odour concentration absolute: 0.014 ppm 50% recognition: 0.023 ppm 100% recognition: 0.046 ppm Odour index 100% recognition: 114 347 (Hellman & Small 1974).
Boiling point, °C	129.4 (MITI 1992)
pKa	5.95 (Sangster 1989)
Log octanol/water coefficient, log Pow	1.11 (Sangster 1989)
Henry's law constant, Pa x m³/mol	2.901 calc. (Yaws et al. 1991)
Total degradation in water	Biodegradation: 57.6% by BOD (on the upward trend) period: 21d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
LD50 values to birds in oral exposure, mg/kg	> 1000 orl-Agelaius phoeniceus > 1000 orl-Sturnus vulgaris > 1000 orl-Coturnix coturnix > 1000 orl-Passer domesticus (Schafer et al. 1983)
Other information about water organisms	Tetrahymena pyriformis, 1002.5 mg/l, EC50, grw, 2.5 d (Schultz et al. 1987).

1402 • 3-Methylpyridine 108-99-6

Synonyms	β-Picoline
Sumformula of the chemical	C6H7N
pKa	5.65 (Sangster 1989)
Log octanol/water coefficient, log Pow	1.2 (Sangster 1989)
LD50 values to birds in oral exposure, mg/kg	1000 orl-Agelaius phoeniceus > 1000 orl-Sturnus vulgaris 1000 orl-Coturnix coturnix 1000 orl-Passer domesticus (Schafer et al. 1983)
Other information about water organisms	Tetrahymena pyriformis, 862.4 mg/l, 2.5 d, EC50, grw (Schultz et al. 1987).

MNO

1403• N-Methylpyrrole 96-54-8

Sumformula of the chemical	C5H7N
EINECS-number	2025137
Water solubility, mg/l	> 3000 (MITI 1992)
Boiling point, °C	112–115 (MITI 1992)
Total degradation in water	Biodegradation: 78% by BOD period: 14d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

1404 • 2-Methylquinoline 91-63-4

Other information about water organisms	LC50 (96hr), 26.4 mg/l, Xenopus laevis (Eldridge & Echevarria 1978).

1405 • 6-Methylquinoline 491-35-0

LC50 values to crustaceans, mg/l	11	48hr, Daphnia magna (Herbes & Beauchamp 1977)

1406 • α-Methylsiloxy-ω-trimethylsilyl-poly(hydro=methylsiloxy) 72319-10-9

Water solubility, mg/l	> 100	(MITI 1992)
Melting point, °C	< -10	(MITI 1992)
Boiling point, °C	> 300	(MITI 1992)
Bioconcentration factor, fishes	< 0.8–6.2 < 7.6–23	6w, Cyprinus carpio, conc 1 mg/l 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 500	48hr, Oryzias latipes (MITI 1992)

MNO

1407 • α-Methylstyrene 98-83-9

Sumformula of the chemical	C9H10
EINECS-number	2027050
Boiling point, °C	161–162 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

Bioconcentration factor, fishes	15–140 8w, Cyprinus carpio, conc 0.3 mg/l 12–113 8w, Cyprinus carpio, conc 0.03 mg/l (MITI 1992)
Other information about bioacculumation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	6.8 48hr, Oryzias latipes (MITI 1992)

1408 • Methyltrichlorostannane 993-16-8

Synonyms	Methyl trichloride stannane
EC50 values to algae, mg/l	0.078 72hr, rpd, Skeletonema costatum (Walsh et al. 1985)

1409 • Metolachlor 51218-45-2

Use	Herbicide.
Half-life in soil, days	42 (Li et al. 1990)
Effects on plants	Metolachlor reduced germination ofdodder (Cuscuta australis) seeds by 51% and reduction of stem elongation was 14% at a concentration of 0.050 mg/ml (seeds/seeds with shoots were placed to Petri dishes on filter paper where the herbicide solution was added) (Giannopolitis 1979).

1410 • Metoxuron 19937-59-8

Synonyms	3-(3-Chloro-4-methoxyphenyl)-1,1-dimethylurea Dosanex * N-(3-Chloro-4-methoxyphenyl)-N', N'-dimethylurea
Sumformula of the chemical	C10H13ClN2O2
Products containing the chemical	Dosanex * metoxuron 800 g/kg (PESREG)
Use	Active ingredient in herbicides.
Instructions for handling	Approx. 4 years when stored in orginal containers in a dry place and at an annual average temperature not exceeding 25 °C. (Dosanex *) (PESREG)
State and appearance	Colourless crystalline powder. Nearly colourless to beige amorphous powder (techn. pr.) Beige to light brown microgranules (Dosanex *) (PESREG)
Odour	Odourless Practically odourless (techn. pr.) (PESREG)
Molecular weight	228.7
Vapour pressure, mmHg	0.000000035 mmHg, 20 °C (Geissbühler et al. 1975)
Water solubility, mg/l	678 at 24 °C, Geissbühler et. al 1975
Melting point, °C	127 (PESREG)
Boiling point, °C	> 250 °C, 760 torr (PESREG)
Log octanol/water coefficient, log Pow	1.56–1.64 (PESREG)

Adsorption/desorption	The adsorption behaviour of metoxuron was investigated in 10 different soil types. The Freundlichs adsorption constants (Ka) range between 2 and 65.5 ppm for soils with 1.1 to 32.5% organic matter content (PESREG). Soluble in acetone, cyclohaxanone and hot ethanol; moderately soluble in ether, benzene and toluene; practically insoluble petroleum spirit (Pesticide Manual 1987).
Photochemical degradation in water	Metoxuron is degraded quickly by sunlight and UV light in solution or when applied on glass and thin layer chromatography plates, as well as on soil surfaces (Wisson et. al 1976). Sunlight irradiation of metoxuron in water caused a rapid decomposition (65% within 58 hours of sunlight), whereas the a.i. protected from light was fairly stable (loss of 4%) (PESREG).
Hydrolysis in water	The hydrolysis half-life of metoxuron in buffer solutions (5 ppm, 50 °C) was 20 days (pH 5), 24 days (pH 7) and 30 days (pH 9). The major hydrolysis product was o-chloro-p-anisidine (40% at pH 5, over 80% at pH 7 and 9). Monomethylmetoxuron and desmethylmetoxuron were identified as hydrolysis products. There were two half-life-times (t1, t2) to metoxuron (5 ppm) at 70 °C: *t1 (days)* / *t2 (days)* at pH 5: 0.2–0.4 / about 1 at pH 7: 0.5–0.8 / about 3 at pH 9: about 1 / about 5 (PESREG) Half-life periods of metoxuron (5 ppm) in aqueous buffer solution: *pH* / *at 50 °C (days)* / *at 20 °C (months)** 3 / 18 / 11 5 / 21 / 13 7 / 24 / 15 9 / > 30 / > 20 11 / 26 / 16 * calc. from values at 50 °C (Wisson et al. 1976)
Aerobic degradation in water	The degradation of metoxuron (at 22 °C) in natural surface water and sediment has been investigated. The half-lives were 230 days (sand, lime 24.2%) and 60 days (sand, lime 1.1%). The metabolite product was monomethylmetoxuron (PESREG).
Degradation and transformation products	monomethylmetoxuron (MMM) desmethylmetoxuron (DMM) o-chloro-p-anisidine (OCPA) (PESREG).
LD50 values to mammals in oral exposure, mg/kg	3353 orl-rat male (PESREG) 1820 orl-rat male, Dosanex * (PESREG) > 1000 orl-rat, metabolite MMM 4600 orl-rat male, metabolite DMM 770 orl-rat male, metabolite PCPA (PESREG)
LD50 values to mammals in non-oral exposure, mg/kg	2000 idr-rat male, Dosanex * (PESREG) 340 ipr-rat male (PESREG) 300 about 300, ivn-rat male (PESREG)
LC50 values to mammals in inhalation exposure, mg/m³	14.7 mg/l, 4hr, inh-rat, Dosanex * (PESREG)
Other information about birds	NOEL of metoxuron for chickens was > 1250 ppm (PESREG).

MNO

Effects on bees	LD50, > 0.2 mg/g bee, oral LD50, > 0.16 mg/g bee, topical LD50, > 2.5 mg/g bee, deposit (PESREG)
Effects on plants	0.15 kg a.i. metoxuron /ha was applied with a sprayer to blackgrass (Alopecurus myosuroides Huds.) at the 2- to 3-leaf stage —a decrease in mean fresh weight of plants (Blair 1978).
Effects on microorganisms	Dosanex (8 ppm and 16 ppm) has no adverse effects on the respiration and ammonification-nitrification processes in the soil (PESREG).
EC50 values to algae, mg/l	0.064 96hr, grw, Scenedesmus subspicatus (OECD 201, PESREG)
EC50 values to crustaceans, mg/l	215.6 24hr, imb, Daphnia magna (OECD, PESREG)
LC50 values to fishes, mg/l	40 96hr, Rasbora heteromorpha (Tooby et al. 1975) 19.8 96hr, Salmo gairdneri (Pesticide Manual 1983) 81 96hr, Cyprinus carpio 18.9 96hr, Salmo gairdneri (PESREG)

1411 • Metribuzin

21087-64-9

Synonyms	4-Amino-6-tert-butyl-3-methylthio-1,2,4-triazin-5(4H)-one 4-Amino-6-(1,1-dimethylethyl)-3-(methylthio)-1,2,4-triazin-5(4H)-one
Use	Active ingredient in herbicides. Effective in the control of broad leafed and grassy weeds encountered in the growing of potatoes and tomatoes.
State and appearance	White crystalline solid.
Melting point, °C	125–126.5 °C
Log soil sorption coefficient, log Kom	1.98 (Sabljic 1987)
Half-life in soil, days	37 (Li et al. 1990)
Other information about degradation	Metribuzin has been shown to undergo nonbiological degradation in four Manitoba soils under dry conditions at 15 °C, and the rate law describing this degradation has been shown to be somewhat less than first order. Calculated times for 50% loss (at a "normal" application rate of 1.8 ppm metribuzin) vary with soil type from approximately 90–115 days for Red River, Almasippi, and Stockton soils to three times this period for Newdale soil. At higher application rates, half lives are somewhat longer (Webster et al. 1978).
LD50 values to mammals in oral exposure, mg/kg	1936–1986 orl-rat (Anon. 1976)
LD50 values to mammals in non-oral exposure, mg/kg	2000 skn-rat (Anon. 1976)
LD50 values to birds in oral exposure, mg/kg	> 100 orl-Agelaius phoeniceus > 100 orl-Passer domesticus > 100 orl-Quiscalus quiscula > 100 orl-Molothrus ater (Schafer et al. 1983)
Effects on plants	Soil was amended to give 2.0 ppm by weight of soil of metribuzin —atrazine-susceptible lamb's-quarters (Chenopodium album L.) were killed soon after germination and emergence (Jensen et al. 1977). Metribuzin was applied as foliar sprays to the tomatoes grown under growth room conditions. Shoot dry weights for 6-week-old tomatoes, 2 weeks after treatment with 0.25 kg/ha metribuzin ranged from 78 to 85% of the control (Stephenson et al. 1980).

MNO

LC50 values to fishes, mg/l	140	96hr, Rasbora heteromorpha (Tooby et al. 1975)
	76	act, Salmo gairdneri
	80	act, Lepomis macrochirus (Pesticide Manual 1983)

1412 • Mevinphos

7786-34-7

Synonyms	2-Methoxycarbamoyl-1-methylvinyldimethylphosphate Phosdrin	
Use	Active ingredient in insecticides, acaricide.	
Molecular weight	224.17	
Boiling point, °C	99–103	
LD50 values to mammals in oral exposure, mg/kg	3	orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	4.2	skn-rat (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	3	orl-bwd
	4.6	orl-dck (Lewis & Sweet 1984)
	1.78	orl-Agelaius phoeniceus
	3.90–7.50	orl-Sturnus vulgaris
	23.7	orl-Coturnix coturnix
	1.78	orl-Passer domesticus
	4.22	orl-Quiscalus quiscula
	4.22	orl-Columba livia (Schafer et al. 1983)
LD50 values to birds in dermal exposure, mg/kg	11	skn-dck (Lewis & Sweet 1984)
LC50 values to crustaceans, mg/l	0.00043	96hr, Simocephalus serrulatus
	0.00016	96hr, Daphnia pulex (Sanders & Cope 1966)
	0.0028	96hr, Gammarus fasciatus (Sanders 1972)
	0.0002	act, Daphnia pulex (Kenaga 1979)
LC50 values to fishes, mg/l	0.012	Salmo gairdneri
	0.023	act, Lepomis macrochirus (Kenaga 1979)
	0.041	24hr, Lepomis macrochirus
	0.034	24hr, Salmo gairdneri (Edwards 1977)
	0.07	96hr, Lepomis macrochirus (Verschueren 1983)

1413 • Mirex

2385-85-5

Synonyms	1,1a,2,3a,4,5,5a,5b,6-Dodecachlorooctahydro-1,3,4-methano-1H-cyclobuta(cd)pentalene
Use	Insecticide; flame-retardant coatings.
State and appearance	Snow-white, free-flowing crystalline solid.
Molecular weight	546

MNO

Water solubility, mg/l	0.2 24 °C
Log octanol/water coefficient, log Pow	6.89 (Mackay 1982)
Bioconcentration factor, mollusca	34200–73700 (Verschueren 1983)
Bioconcentration factor, crustaceans	16860–71400 (Verschueren 1983)
Bioconcentration factor, algae	12200 (Verschueren 1983)
LD50 values to mammals in oral exposure, mg/kg	235 orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	800 skn-rbt (Lewis & Sweet 1984) 600 ukn-rat (Virtanen & Nuuja 1987)
Other information about mammals	Deer mouse: LDfr ≤ 1225 mg/kg, ALD 1600 mg/kg (Virtanen & Nuuja 1987). After spraying Mirex there was a quick increase in Mirex concentrations in striped skunk and in red fox. In aquatic ecosystem Mirex moved slower and the concentrations did not increase until a year after spraying. Mirex itself is not very poisonous to mammals; its degradation products kepone, monohyrdomirex and dihydromirex are the poisonous ones (Virtanen & Nuuja 1987).
Carcinogenicity	Carcinogenic to rat (Virtanen & Nuuja 1987).
LD50 values to birds in oral exposure, mg/kg	2400 orl-dck (Lewis & Sweet 1984) > 100 orl-Agelaius phoeniceus > 562 orl-Sturnus vulgaris (Schafer et al. 1983)
LOEC values to fishes, mg/l	0.013 rpd, chr, Pimephales promelas (Buckler et al. 1981)
Effects on the physiology of water organisms	Salmo gairdneri, 0.0005 mg/g, 180 d, hematological effect (change in various blood parameters such as red blood cell count, hematocrit, and serum osmolarity) (Chen et al. 1986).

1414 • Mitrol 10 * 57520-17-9

Active ingredients	Guazatine * 10%
Use	Pesticide.
LC50 values to crustaceans, mg/l	21 96hr, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	150 96hr, Alburnus alburnus (Linden et al. 1979)

1415 • Mitrol 48 * 75797-91-0

Active ingredients	Alkyldimethylbenzyl ammoniumchloride * 400 g/l
Use	Pesticide.
LC50 values to crustaceans, mg/l	0.9 96hr, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	5.5–6.5 96hr, Alburnus alburnus (Linden et al. 1979)

1416 • Molinate

2212-67-1

Synonyms	S-Ethyl-hexahydro-1H-azepine-1-carbothioate S-Ethyl-1-hexamethylene-iminothiocarbamate	
Use	Herbicide.	
Molecular weight	187.33	
Water solubility, mg/l	880	
Boiling point, °C	117	
LD50 values to mammals in oral exposure, mg/kg	501	orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	3536	skn-rbt (Lewis & Sweet 1984)
Effects on plants	Seeds of selected rice (Oryza sativa L.) lines were planted to sand which was then saturated with a solution containing the commercial formulation of molinate (6 EC). The growth of shoots was strikingly affected by molinate. Entries showed the most variation in response when compared at the 2 ppmw molinate concentration with the response ranging from slight stimulation (127%) to severe inhibition (8%). At the 1 ppmw molinate concentration most entries showed slight stimulation or only slight inhibition; while at the 4 ppmw there was severe inhibition of most entries (Richard & Baker 1979). Molinate was used in the greenhouse at dose of 0.5 kg/Ha incorporated 6 cm deep in a silt loam. Purple nutsedge (Cyperus rotundus L.) tubers were planted 5 cm deep. Molinate stimulated the number of sprouts produced per sproute tuber but those sprouts were short, had swollen tips and did not reach the soil surface (Rincon & Warren 1978).	
LC50 values to crustaceans, mg/l	0.6 0.4 0.6 0.3	48hr, Daphnia magna 48hr, Asellus brevicaudus (Kemp et al. 1973) 96hr, Daphnia magna 96hr, Gammarus fasciatus (Sanders 1970)
LC50 values to fishes, mg/l	0.48 0.18 16.4 29 30 0.2	48hr, Lepomis macrochirus (Kemp et al. 1973) 21 d, Cyprinus carpio (Kawatsu 1977) 96hr, Gambusia affinis (Chaiyrach et al. 1975) 96hr, Lepomis macrochirus 96hr, Carassius auratus 96hr, Salmo gairdneri (Anon. 1972)

1417 • Mono(2,2-dimethylhydrazide) succinic acid

1596-84-5

Synonyms	Succinic acid 2,2-dimethylhydrazide Alar Aminozide Butenedioic acid mono(2,2-dimethylhydraxide) Daminozide N-Dimethyl amino-β-carbamyl propionic acid Dimethylamino succinamic acid Succinic 1,1-dimethyl hydrazide
Sumformula of the chemical	C6H12N2O3

Use	A plant growth regulator currently being used on a variety of food crops and fruit trees.	
Molecular weight	160.2	
Half-life in soil, days	3–4	days, under greenhouse conditions (Verschueren 1983)
Other information about degradation	Microbial degradation is the major route of dissipation. Major degradation product is CO2, which is liberated in amounts of up to 84% in 14 days (Verschueren 1983).	
LD50 values to mammals in oral exposure, mg/kg	6300 8400	orl-mus orl-rat (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	8400	ukn-mam (Sweet 1987)
LDLo values to mammals in non-oral exposure, mg/kg	62	ipr-mus (Sweet 1987)
TDLo values to mammals in oral exposure, mg/kg	2600 182	orl-mus, 62 w, tumorigenic orl-rat, 2 yr, tumorigenic (Sweet 1987)
Carcinogenicity	NCI carcinogenesis bioassay (feed); clear evidence: mouse, rat (Sweet 1987).	
LD50 values to birds in oral exposure, mg/kg	> 100	orl-Agelaius phoeniceus (Schafer et al. 1983)
LC50 values to crustaceans, mg/l	98.5	48hr, water flea (Pesticide Manual 1983)
LC50 values to fishes, mg/l	423 149	96hr, Lepomis macrochirus 96hr, Salmo gairdneri (Pesticide Manual 1983)
Other information	Since the chemical is applied as a foliar spray, direct soil contamination results. Also since alar is water soluble, it can be washed off the plants onto the soil (Verschueren 1983).	

1418 • N-Mono(or di)methylphenyl-N'-mono(or di)methylphenyl-1,4-phenylenediamine

27417-40-9 *m=n=1
70290-05-0 *m=1, n=2
28726-30-9 *m=n=2

Sumformula of the chemical	C20H20N2 *m=n=1, 16.3%; C21H22N2 *m=1, n=2, 49.4%; C22H24N2 *m=n=2, 34.3%	
Water solubility, mg/l	< 10	(MITI 1992)
Melting point, °C	< -30	(MITI 1992)
Boiling point, °C	200–260	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

MNO

Bioconcentration factor, fishes	3760–9800 4210–9950 3340–8530 5290–14600 6330–15200 7710–14600	8w, Cyprinus carpio, conc 0.1 mg/l 8w, Cyprinus carpio, conc 0.1 mg/l 8w, Cyprinus carpio, conc 0.1 mg/l 8w, Cyprinus carpio, conc 0.01 mg/l 8w, Cyprinus carpio, conc 0.01 mg/l 8w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
LC50 values to fishes, mg/l	11.6	48hr, Oryzias latipes (MITI 1992)

1419 • Mono sodium 4-amino-5-hydroxy-1,3-naphthalene disulfonate 52789-62-5

Water solubility, mg/l	> 100000 (MITI 1992)	
Total degradation in water	Biodegradation: 1.2% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.8 < 8.0	6w, Cyprinus carpio, conc 2 mg/l 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 500	48hr, Oryzias latipes (MITI 1992)

1420 • Monoallylamine 107-11-9

Synonyms	2-Propenylamine 3-Amino-1-propene	
Sumformula of the chemical	C3H7N	
pKa	9.51	(Sangster 1989)
Log octanol/water coefficient, log Pow	0.03	(Sangster 1989)
Chemical oxygen demand, g 02/g	2.12	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0	5 days (Bridie et al. 1979)
LC50 values to fishes, mg/l	27 60	96hr, Carassius auratus 24hr, Carassius auratus (Bridie et al. 1979)

1421 • Monobutylnaphthalene sulfonic acid and sodium salt 25638-17-9

Sumformula of the chemical	C14H1503SNa
Water solubility, mg/l	> 20000 (MITI 1992)

Total degradation in water	Biodegradation: 1% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.13 < 1.5	6w, Cyprinus carpio, conc 2 mg/l 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
LC50 values to fishes, mg/l	360	48hr, Oryzias latipes (MITI 1992)

1422 • Monochlorodehydroabietic acid 57055-38-6

LC50 values to fishes, mg/l	0.6	96hr, Salmo gairdneri (Leach & Thakore 1975)

1423 • Monochlorohydroquinone 615-67-8

LC50 values to crustaceans, mg/l	0.017	act, Daphnia magna (Verschueren 1983)
LC50 values to fishes, mg/l	0.19	act, Pimephales promelas (Verschueren 1983)

1424 • Monocrotophos 6923-22-4

Synonyms	Dimethyl-1-methyl-2-(methylcarbamoyl)vinylphosphate Azodrin Dimethylphosphate of 3-hydroxy-N-methyl-cis-crotonamine- 0,0-Dimethyl-0-(2-methylcarbamoyl-1-methyl-vinyl)phosphate
Sumformula of the chemical	C7H14NO5P
Use	Systemic insecticide; acaricide.
Molecular weight	223.19
Total degradation in water	Persistence in riverwater in a sealed glass jar under sunlight and artificial fluorescent light – initial conc. 0.010 mg/l: *% of original compound found after* 1hr: 100; 1 wk: 100; 2 wk: 100; 4 wk: 100; 8 wk: 100 (Eichelberger & Lichtenberg 1971).
LD50 values to mammals in oral exposure, mg/kg	8–23 orl-rat (Anon. 1976)
LD50 values to mammals in non-oral exposure, mg/kg	354 skn-rbt (Anon. 1976)
Other information about mammals	ALD = 28 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987). LDfr = 37.5 mg/kg/day, subacute, deer mouse.

MNO

LD50 values to birds in oral exposure, mg/kg	1 orl-Agelaius phoeniceus 3.16–5.62 orl-Sturnus vulgaris 4.22 orl-Coturnix coturnix 13.3 orl-Passer domesticus 17.8 orl-Quiscalus quiscula 13.3 orl-Columba livia 1.33 orl-Quelea quelea (Schafer et al. 1983)
LC50 values to crustaceans, mg/l	4.46 48hr, rpd, Macrobrachium lamarrei (Nagabhushanam et al. 1983) 0.24 96hr, Acartia tonsa (Khattat & Farley 1976) 1.59 96hr, Macrobrachium lamarrei (Omkar & Shukla 1985)
LC50 values to fishes, mg/l	4.9 act, Salmo gairdneri (Kenaga 1979) 12 24hr, Salmo gairdneri (Pesticide Manual 1983) 450 96hr, Rasbora heteromorpha (Tooby et al. 1975)
Effects on the physiology of water organisms	Barbus conchonius, 60–120 d, 0.053 mg/l, histological effect (Kumar & Pant 1988). Nostoc linckia, 20 d, 5 mg/l, effect on nitrogen fixation (Megharaj et al. 1988).
Other information about water organisms	LC100 (96hr) 18.6 mg/l, Sarotheredon aureus (Mustafa et al. 1982).

1425 • Monoethyl adipate 626-86-8

Synonyms	Adipic acid mono ethyl ester
Water solubility, mg/l	76000 (MITI 1992)
Melting point, °C	20 (MITI 1992)
Log octanol/water coefficient, log Pow	0.91
Total degradation in water	Biodegradation: 81–87% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

1426 • Monoethyl biphenyl 40529-66-6

Boiling point, °C	285–286 (MITI 1992)
Total degradation in water	Biodegradation: 42–100% by BOD (on the upward trend) period: 14d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

MNO

1427 • Monofluoroacetic acid 144-49-0

Molecular weight	78.05	
LD50 values to mammals in oral exposure, mg/kg	4.68 0.468	orl-rat orl-gpg (Lewis & Sweet 1984)
LDLo values to mammals in non-oral exposure, mg/kg	0.05	unk-dog (Lewis & Sweet 1984)
LOEC values to algae, mg/l	0.0004 0.055	rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976) rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
Other information about water organisms	LOEC 31 mg/l, rpd, schr, Entosiphon sulcatum (Bringmann & Kühn 1980a).	

1428 • Monolauryl phosphoric ester 2627-35-2

Sumformula of the chemical	C12H27O4P	
Melting point, °C	60–90	(MITI 1992)
Total degradation in water	Biodegradation: 79–88% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

1429 • Monolinuron 1746-81-2

Synonyms	3-(4-Chlorophenyl)-1-methoxy-1-methylurea	
Use	Herbicide.	
Molecular weight	214.67	
LD50 values to mammals in oral exposure, mg/kg	1800 500	orl-rat orl-dog (Lewis & Sweet 1984)
LOEC values to algae, mg/l	0.14	Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to crustaceans, mg/l	1.3	96hr, Daphnia magna (Knapek & Lekola 1974)
LC50 values to fishes, mg/l	3.1 12.9 54 105	96hr, Salmo trutta m. fario 96hr, Cyprinus carpio (Knapek & Lekola 1974) 96hr, Sarotheredon aureus 96hr, Channa punctata (Rao & Dad 1979)
Other information about water organisms	LC50 (96hr), 24.2 mg/l, Mosquito larvae (Knapek & Lekola 1974).	

1430 • Monomethylamine hydrochloride 539-51-1

Sumformula of the chemical	CH6NCl	
Water solubility, mg/l	> 10000 mg/l (MITI 1992)	

MNO

Melting point, °C	225–226 (MITI 1992)
Boiling point, °C	225–230 15 mmHg (MITI 1992)
Total degradation in water	Biodegradation: 42–44% by BOD period 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

1431 • Monomethylhydrazine 60-34-4

Synonyms	MMH Methylhydrazine Hydrazomethane 1-Methylhydrazine
Sumformula of the chemical	CH6N2
Use	Rocket fuel and intermediate in chemical synthesis.
Molecular weight	46.07
Specific gravity (water=1)	0.874
Vapour pressure, mmHg	49.6 25 °C
Melting point, °C	52.4
Boiling point, °C	87.5
Flashing point, °C	8.3 (Sax 1986) 70 open cup (Sax 1986)
Other physicochemical properties	Oxidants like HOOH or HNO3 separate from oxidizing materials. Ignites spontaneously on contact with fluorine, chlorine trifluoride, nitrogen tetroxide, and fuming nitric acid. May explode in contact with metallic oxides (Sax 1986). Flammability: Quite flammable liquid. May ignite spontaneously in air with porous materials such as earth, asbestos, wood, or cloth or when spilled. Spontaneous ignition can occur with oxidant like hydrogen peroxide or nitric acid. Vapour is heavier than air and may flash back to source of ignition (Sax 1986). Explosiveness: Vapour forms explosive mixtures over wide range in air. Explosive at high temperatures (Sax 1986). Soluble.
Other reactions in air	Decomposition of monomethylhydrazine in air is very complex. Some primary reaction products decompose into secondary products. A total of 17 decomposition products have been identified by the Naval Research Laboratory. The decomposition rate depends on surfaces in contact with the reactants and the reaction container's surface-to-volume ratio. Main autoxidation products in air are HCHO, methylhydrazone, CH4, N2, and water. The half-life is 2 to 7hr. The tropospheric half-life due to reaction with HO-radical is approximately 3hr (Sax 1986).
Total degradation in water	In vitro, monomethylhydrazine is susceptible to air oxidation. It is thought to degrade chemically via a methyldiazene, and extremely unstable monoalkyl azo compound known to decompose (in the presence of oxygen) via a free radical mechanism to methane and nitrogen gas. – In hard water, hydrazine compounds at 100 mg/l show considerable coordination with calcium and other hard water ions and reduce the dissolved oxygen content. – In acidic media, monomethylhydrazine is oxidized by a variety of oxidizing agents to CH3OH, N2, and H2 (Sax 1986).

LD50 values to mammals in oral exposure, mg/kg	70.7 orl-rat 22.1 orl-ham 57 orl-mus 33 orl-rat 33 orl-mus (Sax 1986)
LD50 values to mammals in non-oral exposure, mg/kg	183.4 skn-rat 239.4 skn-ham 21.2 ipr-ham 28 ipr-rat 17 ivn-rat 35 scu-rat 32.3 ipr-mus 25 scu-mus 33.2 ivn-mus 12 ivn-dog 95 skn-rbt 12 ivn-rbt 48 skn-gpg (Sax 1986)
LC50 values to mammals in inhalation exposure, ppm	74 ihl-rat, 4hr 56 ihl-mus, 4hr 96 ihl-dog, 1hr 82 ihl-mky, 1hr 143 ihl-ham, 4hr (Sax 1986)
TDLo values to mammals in oral exposure, mg/kg	10000 orl-mus, 1Y-C, tumorigenic 3000 orl-ham, 47W-C, tumorigenic (Sax 1986)
TDLo values to mammals in non-oral exposure, mg/kg	100 ipr-rat, 6-15d preg, teratogenic 50 ipr-rat, 6-15d preg, teratogenic 72 ipr-mus, 8W-I, tumorigenic (Sax 1986)
Health effects	Direct contact: Vapours attact eyes and respiratory system. Liquid is corrosive to skin. Monomethylhydrazine was absorbed rapidly through the shaved skin of dogs when a solution equivalent to 3.6 mg/kg was applied. General sensation: Acute toxic systems in rats, mice, dogs, and monkeys were irritation of the nose and eyes, emesis, ataxia, and convulsions. Methemoglobinemia is a major toxic effect of monomethylhydrazine. Humans exposed to monomethylhydrazine concentrations of 90 ppm for 10 minutes experienced a slight tickling sensation of the nose, slight nasal drip, mild or moderate eye irritation, and/or an unpleasant taste sensation. The odour was less noticeable or offensive to most subjects than 50 ppm NH3. Acute hazard level: Vapours very toxic, promptly attacking eyes and respiratory system. More toxic than hydrazine. Chronic hazard level: Dogs are the most sensitive species to monomethylhydrazine, and chronic inhalation studies with dogs and monkeys showed that 1 ppm monomethylhydrazine, approximate the 'no effect level'. No organ-specific or generalized toxic symptoms were seen in rats and mice chronically exposed to monomethylhydrazine at the following levels: 29 w, at 0.2 ppm continuously, or 0.2 ppm intermittently or 1 ppm intermittently. There was a small but significant depression in weight gain in the two highest exposure rat groups; however chronic dosing of animals shows that it accumulates in the body (Sax 1986).
Carcinogenicity	Carcinogenic to Syrian golden hamsters administered 0.01% in drinking water for life (Sax 1986).

Monome

Mutagenicity	Positive in in vitro studies, in bacteria, and in mice (Sax 1986). Mutagen data: mmo, sat, 0.002 mmol/plate, 48hr; mma, sat, 0.001 ml/plate; dnd, hmn, fbr, 116 pmol; dns, rat, lng, 0.001 mmol/l; dlt, rat, ipr, 1075 mg/kg, 5D-I; dns, ham, ovr, 0.001 mmol/l; dns, ham, lng, 0.001 mmol/l (Sax 1986).
Teratogenicity	Positive in mice given 100 mg/kg orally on days 8–12 of gestation and in a rabbit given 200 mg/kg on day 14. Positive in toad embryos exposed to 10 mg/l (Sax 1986).
LC50 values to fishes, mg/l	2.58 sft, 96hr, Poecilia reticulata 3.26 hrd, 96hr, Poecilia reticulata (Slonium 1977)

1432 • Mordant Black-7 3618-60-8

Sumformula of the chemical	C16H10O6N2NaSCl
Water solubility, mg/l	> 1000 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.34–0.96 6w, Cyprinus carpio, conc 0.4 mg/l < 3.3–4.3 6w, Cyprinus carpio, conc 0.04 mg/l (MITI 1992)
LC50 values to fishes, mg/l	32 48hr, Oryzias latipes (MITI 1992)

1433 • Morpholine 110-91-8

Synonyms	Tetrahydro-1,4-oxazine
Use	Solvent.
Odour	Quality: fishy, amine Hedonic tone: unpleasant Threshold odour concentration absolute: 0.01 ppm 50% recognition: 0.07 ppm 100% recognition: 0.14 ppm Odour index 100% recognition: 65 857 (Hellman & Small 1974).
Melting point, °C	-4.9 (MITI 1992)
Boiling point, °C	128.9 (MITI 1992)
Volatilization	Relative volatility (nBuAc=1) = 0.80

Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.3–0.65 6w, Cyprinus carpio. conc 5 mg/l < 2.8 6w, Cyprinus carpio, conc 0.5 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	1050 orl-rat
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 310 mg/l (Bringmann & Kühn 1980a)
LC50 values to algae, mg/l	28 rpd, schr, Selenastrum capricornutum (Calamari et al. 1982)
LOEC values to algae, mg/l	1.7 rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976) 4.1 rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
LC50 values to crustaceans, mg/l	119 24hr, Daphnia magna (Calamari et al. 1982)
LC50 values to fishes, mg/l	350 96hr, Lepomis macrochirus 400 96hr, Menidia audens (Dawson et al. 1977) 180 96hr, Salmo gairdneri (Calamari et al. 1980) 240 48hr, Oryzias latipes (MITI 1992)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 4.1 mg/l protozoa (Entosiphon sulcatum): 12 mg/l (Bringmann & Kühn 1980a)

1434 • MTBE

1634-04-4

Synonyms	2-Methoxy-2-methylpropane
Sumformula of the chemical	C5H12O
Use	Octane booster for unleaded gasoline up to 7% by volume. Manufacture of isobutene.
State and appearance	Colourless liquid
Odour	Camphor like.
Molecular weight	88.15
Density, kg/m³	740
Conversion factor, 1 ppm in air=	3.6
Conversion factor, 1 mg/m³ in air=	0.278
Vapour pressure, mmHg	414 (38 °C)
Water solubility, mg/l	40000 43000
Melting point, °C	-110

MNO

Boiling point, °C	55
Log octanol/water coefficient, log Pow	1.3 0.94 (Sangster 1989)
Mobility	In the ground MTBE moves faster than other components of gasoline. Dissolvable to alcohols and ethers flash point: -28 °C explosion limits: 1.64-8.4%-vol self ignition temperature: 460 °C.
Other reactions in atmosphere	Main oxidation products: tert-butylformiate, acetone methyl-radical.
Half-life in air, days	3.5
Half-life in water, days	0.4 volatilises from water surface to atmosphere
LD50 values to mammals in oral exposure, mg/kg	4000 (Laiho 1989)
LC50 values to mammals in inhalation exposure, mg/m³	80000 ihl-rat (Laiho 1989)
Health effects	Narcotic.
LC50 values to fishes, mg/l	760 96hr (Laiho 1989)

1435 • N-2404 328-04-1

Other information about mammals	ALD = 62.0 mg/kg, act, orl, deer mouse; LDfr = 100 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

1436 •4-(N, N-Dimethylamino)-1,2-dithiolane 1631-58-9

Sumformula of the chemical	C5H11NS2
Water solubility, mg/l	> 2000 (MITI 1992)
Melting point, °C	177.2 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	29–59 8w, Cyprinus carpio, conc 0.00156 mg/l 40–64 8w, Cyprinus carpio, conc 0.000156 mg/l (MITI 1992)
LC50 values to fishes, mg/l	0.207 48hr, Oryzias latipes (MITI 1992)

1437 • 2-(N-Phenylamino)naphthalene 135-88-6

Synonyms	2-Naphthalenamine, N-phenyl-
Sumformula of the chemical	C16H13N
EINECS-number	2052239
Melting point, °C	> 105 (MITI 1992)

Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Bioconcentration factor, fishes	80–290 8w, Cyprinus carpio, conc 0.045 mg/l 60–410 8w, Cyprinus carpio, conc 0.0045 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	1.2 48hr, Oryzias latipes (MITI 1992)

1438 • NAA

86-87-3

Synonyms	1-Naphthaleneacetic acid 1-Naphthyl acetic acid
Use	Herbicide.
Water solubility, mg/l	500 (MITI 1992)
Melting point, °C	131 (MITI 1992)
Log octanol/water coefficient, log Pow	1.2–1.4 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	0.15–0.59 6w, Cyprinus carpio, conc 0.5 mg/l < 1.7–4.2 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
Effects on plants	Aspen plants (Populus tremula) were grown in solutions: 10–4 M (concentration of the solution) —epinastic curvatures, swelling of the stem base, time of survival 22 days (Eliasson 1963).
LC50 values to fishes, mg/l	210 48hr, Oryzias latipes (MITI 1992)

1439 • Nabam

142-59-6

Synonyms	Disodium ethylene-1,2-bidithiocarbamate Disodiumethylenebis(dithiocarbamate) DSE Ethylenebis(dithiocarbamate), disodium salt Ethylenebis(dithiocarbamic acid) sodium salt
Sumformula of the chemical	C4H6N2S4.2Na
Products containing the chemical	Dithane A 40 * 93% Nabam

MNO

Use	Fungicide.	
Molecular weight	256.34	
LD50 values to mammals in oral exposure, mg/kg	395 580	orl-rat (Lewis & Sweet 1984) orl-mus (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	500	ipr-rat (Sweet 1987)
TDLo values to mammals in non-oral exposure, mg/kg	418 194	scu-mus, 6-14d preg. effects on fertility scu-mus, 6-14d preg. effects on embryo or fetus (Sweet 1987)
Mutagenicity	Mutation data: microbial mutation without S9: microorganisms, 1000 ppm (Sweet 1987).	
EC50 values to microorganism, mg/l	102 32	15 min Microtox (Van Leeuwen et al. 1985) Nitrification (Van Leeuwen et al. 1985)
EC50 values to algae, mg/l	2.4	rpd, 96hr, Chlorella pyrenoidosa (Leeuwen et al. 1985)
LC50 values to crustaceans, mg/l	0.44	48hr, Daphnia magna (Leeuwen et al. 1985)
LC50 values to fishes, mg/l	5.8 1.4 1.2	96hr, Poecilia reticulata (Leeuwen et al. 1985) 24hr, Rasbora heteromorpha 48hr, Rasbora heteromorpha (Tooby et al. 1975)
Other information about water organisms	LC50 (12d) 1.75 mg/l, Mercennaria mercennaria (Kemp et al. 1973).	

1440 • Naled

300-76-5

Synonyms	0-(1,2-Dibromo-2,2-dichloroethyl)-0,0-dimethylphosphate	
Use	Insecticide.	
Molecular weight	380.8	
Vapour pressure, mmHg	0.002	20 °C
Boiling point, °C	110	
LD50 values to mammals in oral exposure, mg/kg	250	orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	800 7.7	skn-rat ihl-rat (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	52	orl-dck (Lewis & Sweet 1984)
LC50 values to crustaceans, mg/l	0.33 3.3 0.08 0.18 0.13 2	act, Lepomis macrochirus act, Pimephales promelas Salmo gairdneri (Kenaga 1979) 96hr, Lepomis macrochirus 96hr, Salmo gairdneri (Verschueren 1983) 24hr, Carassius auratus (Pesticide Manual 1983)

MNO

1441 • Naphtha

8030-30-6

LC50 values to crustaceans, mg/l	0.4–2	Daphnia magna (Dennis et al. 1979)
LC50 values to fishes, mg/l	4–21 2–4	96hr, Pimephales promelas 96hr, Lepomis macrochirus (Dennis et al. 1979)

1442 • Naphthalene

91-20-3

Synonyms	Naphthalin Naphthene
Sumformula of the chemical	C10H8
Purity, %	80.2
Use	Moth ball manufacturing; manufacturing of α- and β-naphthols and pesticides and fungicides; asphalt and naphtha constituent. Chemicals; resins; manufacture hydronaphthalene; smokeless powder; insecticide 2842; veterinary; medical.
State and appearance	White flakes or powder.
Molecular weight	128.18
Specific gravity (water=1)	1.162
Vapour density (air=1)	4.42
Vapour pressure, mmHg	1 53 °C 0.23 25 °C
Water solubility, mg/l	30 0.03 25 °C 30 30 °C (MITI 1992)
Melting point, °C	80.2 80.3 (MITI 1992)
Boiling point, °C	217.9 218 (MITI 1992)
Sublimation point, °C	217.9
Flashing point, °C	79
Log octanol/water coefficient, log Pow	3.59 (Anon. 1986) 3.01–4.70 (Sabljic 1987) 3.38 (Chin et al. 1986) 3.36 (Schwarzenbach & Westall 1981) 3.3 (Schwarzenbach et al. 1983) 3.59 (Mackay 1982) 3.35 (Sangster 1989)
Log organic C/water coefficient, log Pcw	3.11 exptl (Schwarzenbach & Westall 1981) 2.91 calcd (Schwarzenbach & Westall 1981)
Henry's law constant, Pa x m³/mol	124.5 calc. (Yaws et al. 1991)
Volatilization	Evaporation from water: calculated half-life (25 °C): 7.15hr (Verschueren 1983).
Other physicochemical properties	Autoignition point: 567 °C. Vapour forms explosive mixtures with air. Highly reactive.

MNO

Total degradation in water	Biodegradation: 2% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).
Other information about degradation	Biodegrades at slow-moderate rate. Half-life in < saturated solution (top meter) is estimated to be 2.9 hours; as a result of evaporative losses. 19% evaporates with first 0.01% of water (Sax 1986). Subject to biodegradation: First degradation product is salicylic acid, next to catechol and b-ketoadipic acid. A second degradation route results in 1,2-naphthoquinone (Sax 1986). Degradation of naphthalene:

ENVIRONMENT	*INIT.CONC. mg/l*	*REDOX-COND.*	*TEMP. °C*	*DEGRADATION %/day*	*REF.*
water	2.48	aerobic	-	99/17	a
water	1–3	aerobic	20	100/8	b
water	1–3	anaerobic	20	0/41	b
water	5	aerobic	25	100/7	c
water	10	aerobic	25	100/7	c
groundwater	10	aerobic	10	28/7	d
groundwater	10	aerobic	10	100/9	d
groundwater	0.45–1.33	aerobic	10–13	100/4	e
groundwater	0.45	aerobic	10–13	95/4	e
groundwater	0.014	aerobic	-	> 99/1	f
sediment	-	anaerobic	30	0/36	g
sediment	-	anaerobic	20–30	0/233	h
soil	0.000042	aerobic	20	0/14	i

a) Battermann 1984
b) Delfino & Miles 1985
c) Tabak et al. 1981
d) Kappeler & Whurmann 1978
e) Jensen et al. 1985
f) Bouwer 1987
g) Delaune et al. 1980
h) Ward & Brock 1976
i) Hutchins & Ward 1984
(Anon. 1987b).

Bioconcentration factor, fishes	12–700 (Verschueren 1983) 36.5–168 8w, Cyprinus carpio, conc 0.15 mg/l 23–146 8w, Cyprinus carpio, conc 0.015 mg/l (MITI 1992)
Bioconcentration factor, crustaceans	4000–6000 (Verschueren 1983)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	1250 orl-rat 580 orl-mus (Lewis & Sweet 1984) 1780 orl-rat 1000 orl-mam (Sax 1986)
LD50 values to mammals in non-oral exposure, mg/kg	150 ipr-mus 969 scu-mus 100 ivn-mus (Sax 1986)

MNO

LDLo values to mammals in oral exposure, mg/kg	400 100 1000 3000	orl-dog (Lewis & Sweet 1984) orl-child orl-cat orl-rbt (Sax 1986)
LDLo values to mammals in non-oral exposure, mg/kg	74	unk-man (Lewis & Sweet 1984)
TDLo values to mammals in non-oral exposure, mg/kg	5925 3500	ipr-rat, 1-15d preg, teratogenic scu-rat, 12W-I, tumorigenic (Sax 1986)
Health effects	Direct contact: Skin; eyes; respiratory tract irritant, occasional (Sax 1986). General sensation: Mothball odour. Metabolites of naphthalene are responsible for the growth of cataracts. – Can be absorbed through skin. Symptoms include nausea, vomiting, headache, diaphoresis, hematuria, hemolytic anemia, fever, hepatic necrosis, conculsions, and coma (Sax 1986). 5–15 g will kill a person. Moderately toxic by ingestion or inhalation (Sax 1986). Chronic hazard level: Possible dermatitis. Slight chronic hazard with ingestion or inhalation. Solid may stay on bottom and provide equilibrium values for prolonged period (Sax 1986). Skin and eye irritation data: skn, rbt, 495, open, mild; eye, rbt, 100 mg, mild (Sax 1986).	
Carcinogenicity	Rat – tumor was negative, in oil (in synthetic diet), six times a week, 10–20 mg until dose of 10 g/rat in food (Sax 1986).	
Mutagenicity	Mutagen data: dnd, mus, ipr, 200 mg/kg (Sax 1986).	
Maximum longterm immission concentration in air for plants, mg/m³	2.5	VDI 2306
Maximum longterm immission concentration in air for plants, ppm	0.5	VDI 2306
Effects on wastewater treatment	Can be toxic to sewage organisms at 2500 ppm (Sax 1986).	
EC50 values to microorganism, mg/l	1154	Biodegradation inhibition (Vaishnav 1986)
LC50 values to crustaceans, mg/l	1 8.6	96hr, Daphnia pulex (Trucco et al. 1983) 48hr, Daphnia magna (LeBlanc 1980)
LOEC values to crustaceans, mg/l	1	bhv, act, Daphnia magna (Whitman & Miller 1982)
LC50 values to fishes, mg/l	1.2 6.08 0.12 0.11 > 0.24 0.51 9	96hr, Oncorhynchus gorbusha (Korn et al. 1979) 96hr, Pimephales promelas (Holcombe et al. 1984) 0d, embryo-larval, Salmo gairdneri 4d, embryo-larval, Salmo gairdneri 0d, embryo-larval, Micropterus salmoides 4d, embryo-larval, Micropterus salmoides (Black et al. 1983) 48hr, Oryzias latipes (MITI 1992)
LOEC values to fishes, mg/l	0.85	rpd, schr, Pimephales promelas (DeGraeve et al. 1982)
NOEC values to fishes, mg/l	0.45	grw, schr, Pimephales promelas (DeGraeve et al. 1982)

MNO

Effects on the physiology of water organisms	Tilapia mossambica, 3.95 mg/l, 4 d, change in enzyme activity (Dange 1986). Macrobrachium kistnensis, 0.5957 mg/l, 10 days, biochemical effect (Sarojini et al. 1987).
Other information about water organisms	LC50 13 mg/l, chr, Chironomus attenuatus LOEC 0.5 mg/l, phy, chr, Chironomus attenuatus LC50 13 mg/l, chr, Tanytarsus dissimilas LOEC 0.5 mg/l, phy, chr, Tanytarsus dissimilas (Darville & Wilhm 1984). 1.8 mg/l, 72hr, fingerling salmon, critical; 4 mg/l, 1hr, Lepomis, death; 20 mg/l, Perca fluviatilis, killed; 11 mg/l, 15 mg/l, minnows, killed (Sax 1986).
Other information	Air pollution: high (Sax 1986). Will produce tastes and BOD in water (Sax 1986).

1443 • 1-Naphthalene carboxaldehyde 66-77-3

Effects on arthropods	LC50, 1 d, > 10.0 mg/l: Aedes aegypti, Aedes taeniorhynchus, Culex quinquefasciatus (Borovsky et al. 1987).

1444 • 2-Naphthalene thiol 91-60-1

Water solubility, mg/l	2.8	(MITI 1992)
Melting point, °C	81	(MITI 1992)
Boiling point, °C	286	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD (disulfidized to di-2-naphthyl disulfide) period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	

1445 • 2,6-Naphthalenedicarboxylic acid 1141-38-4

Sumformula of the chemical	$C_{12}H_8O_4$	
Water solubility, mg/l	2	(MITI 1992)
Melting point, °C	> 300	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period:28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

MNO

Bioconcentration factor, fishes	< 0.6 6w, Cyprinus carpio, conc 0.1 mg/l < 5.2–7.7 6w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioacculation	Confirmed to be non–accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	> 100 48hr, Oryzias latipes (MITI 1992)

1446 • 2-Naphthalenesulfonic acid, 7,7'-(carbonyldiimino)bis-(4- hydroxy- 134-47-4

Synonyms	6,6'-Ureylene-bis(1-naphthol-3-sulfonic acid disodium salt)
Sumformula of the chemical	C21H16N2O9S2
EINECS-number	2051429
Water solubility, mg/l	10000 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.19 6w, Cyprinus carpio, conc 2 mg/l < 1.8 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 1000 48hr, Oryzias latipes (MITI 1992)

1447 • Naphthionic acid sodium salt 130-13-2

Synonyms	1-Naphthalenesulfonic acid, 4-amino-, monosodium salt
Sumformula of the chemical	C10H9NO3S.Na
EINECS-number	2049755
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.6 6w, Cyprinus carpio, conc 10 mg/l < 6.0 6w, Cyprinus carpio, conc 1 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 4000 48hr, Oryzias latipes (MITI 1992)

1448 • γ-Naphthoflavone 604-59-1

Effects on the physiology of water organisms	Salmo gairdneri, 0.63 mmol, 6 d, biochemical effect (change in physiochemical process including glycogen uptake, cholesterol levels and lipid analysis) (Miyauchi & Uematsu 1987).

MNO

1449 • 1-Naphthoic acid 86-55-5

Synonyms	1-Naphthalene carboxylic acid α-Naphthoic acid
Water solubility, mg/l	86 (MITI 1992)
Melting point, °C	161 (MITI 1992)
Total degradation in water	Biodegradation: 40% by BOD (on the upward trend) period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

1450 • 2-Naphthoic acid 93-09-4

Water solubility, mg/l	47 (MITI 1992)
Melting point, °C	184 (MITI 1992)
Total degradation in water	Biodegradation: 79–92% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

1451 • 1-Naphthol 90-15-3

Synonyms	α-Naphthol
Sumformula of the chemical	C10H8O
Use	Dyes, organic synthesis, synthetic perfumes.
State and appearance	Yellow crystals.
Molecular weight	144.18
Vapour pressure, mmHg	1 94 °C
Melting point, °C	96.1 (MITI 1992)
Boiling point, °C	278–280 (MITI 1992)
Log octanol/water coefficient, log Pow	2.71 Anon. 1986 2.31–2.98 (Sabljic 1987) 2.84 (Sangster 1989)
Log soil sorption coefficient, log Kom	3.33 observed (Sabljic 1987) 3.41 calculated (Sabljic 1987)

Total degradation in water	Biodegradation to CO_2 in estuarine waters: turnover time: 41 days (Verschueren 1983). Biodegradation: 96% by BOD period: 14d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	2400	orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	880	skn-rbt (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	> 100	orl-Agelaius phoeniceus (Schafer et al. 1983)
EC50 values to microorganism, mg/l	25.9	DIDHA (Bitton et al. 1986)
EC50 values to algae, mg/l	14	72hr, rpd, Dunaliella bioculata (Heldal et al. 1984)
LC50 values to fishes, mg/l	2.6–3.13 4.24	96hr, Labeo rohita (Tilak et al. 1980) 96hr, Pimephales promelas (Holcombe et al. 1984)

1452 • 2-Naphthol

135-19-3

Synonyms	β-Naphthol	
Sumformula of the chemical	$C_{10}H_8O$	
Use	Dyes; pigments; anti-oxidants for rubber, fats, oils; synthesis of fungicides; pharmaceuticals; perfumes.	
State and appearance	Colourless leaflets.	
Molecular weight	144.18	
Vapour pressure, mmHg	5	145 °C
Water solubility, mg/l	740	25 °C
Melting point, °C	123	(MITI 1992)
Boiling point, °C	285–286	(MITI 1992)
Log octanol/water coefficient, log Pow	2.7	(Sangster 1989)
Total degradation in water	Biodegradation: 68% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992)	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	1960	orl-rat (Lewis & Sweet 1984)
LDLo values to mammals in oral exposure, mg/kg	100	orl-mus, orl-cat (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	> 100	orl-Agelaius phoeniceus (Schafer et al. 1983)

MNO

EC50 values to algae, mg/l	19	pht, 4hr, Selenastrum capricornutum (Millemann et al. 1984)
LC50 values to crustaceans, mg/l	3.5	48hr, Daphnia magna (Millemann et al. 1984)
LC50 values to fishes, mg/l	0.12 3.5 0.08 0.07 6.36 1.77	27 d, Salmo gairdneri 96hr, Pimephales promelas (Millemann et al. 1984) 0d, embryo-larval, Salmo gairdneri 4d, embryo-larval, Salmo gairdneri 0d, embryo-larval, Micropterus salmoides 4d, embryo-larval, Micropterus salmoides (Black et al. 1983)

1453 • 2-Naphthol-3,6-disulfonic acid disodium salt 15883-57-5

Sumformula of the chemical	C10H6O7S2Na2	
Total degradation in water	Biodegradation: 4.4% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.2–0.5 < 2	6w, Cyprinus carpio, conc 1 mg/l 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 1000	48hr, Oryzias latipes (MITI 1992)

1454 • 1-Naphthol-4-sulfonic acid sodium salt 6099-57-6

Sumformula of the chemical	C10H7O3SNa	
Water solubility, mg/l	174000	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 1.3 < 13	6w, Cyprinus carpio, conc 5 mg/l 6w, Cyprinus carpio, conc 0.5 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 1000	48hr, Oryzias latipes (MITI 1992)

1455 • 1,2-Naphthoquinone 524-42-5

LD50 values to birds in oral exposure, mg/kg	75	orl-Agelaius phoeniceus (Schafer et al. 1983)
EC50 values to algae, mg/l	1	72hr, rpd, Dunaliella bioculata (Heldal et al. 1984)

1456 • 1,4-Naphthoquinone 130-15-4

Synonyms	1,4-Naphthalenedione 1,4-Dihydro-1,4-diketonaphthalene α-Naphthoquinone 1,4-Naphthylquinone p-Naphthoquinone
Sumformula of the chemical	$C_{10}H_6O_2$
Purity, %	99.5
Use	Polymerization inhibitor or regulator for polyester resins and rubber; synthesis of dyes and pharmaceuticals; fungicide; algacide.
Odour	Benzoquinonene-like odour, pungent. Odour threshold: lower: 0.02–0.025 ppm (Sax 1986).
Molecular weight	158.11
Specific gravity (water=1)	1.422
Vapour density (air=1)	5.46
Melting point, °C	125
Log octanol/water coefficient, log Pow	1.74
Other physicochemical properties	Slightly soluble in water. Sparingly soluble in cold water, slightly in petroleum ether, freely in hot alcohol, ether, benzene, chloroform, carbon bisulfide, acetic acid (Sax 1986).
Total degradation in water	The potential for degradation or elimination of this compound from a river reach traversed in five days is low (approximately 0.00%). Bottom sediment accumulation estimated to be 13.8 times as great as ambient water concentration (Sax 1986).
Bioconcentration factor, fishes	11.9 (Sax 1986)
LD50 values to mammals in oral exposure, mg/kg	190 orl-rat 400 orl-gpg (Sax 1986)
LD50 values to mammals in non-oral exposure, mg/kg	10 ipr-mus (Sax 1986)
LDLo values to mammals in oral exposure, mg/kg	140 orl-mus (Sax 1986)
TDLo values to mammals in non-oral exposure, mg/kg	5 scu-rat, 1d preg. 800 skn-mus (Sax 1986)
Health effects	Hematological changes, irritant and allergenic activity, and inhibition of biochemical oxidation processes (Sax 1986).
LD50 values to birds in oral exposure, mg/kg	133 orl-Agelaius phoeniceus (Schafer et al. 1983)
EC50 values to algae, mg/l	0.011 72hr, rpd, Dunaliella bioculata (Heldal et al. 1984)
Other information about water organisms	Toxic to algal culture of Selenastrum capricornutum at low concentrations. 59% inhibition of photosynthesis at 0.1% saturated solution, 14% inhibition at 0.01%. Alga Microcystis aeruginosa killed at 100 ppm (Sax 1986). 0.3–0.6 mg/l, 24–48hr, lethal, aerated spring water: Pomoxis nigromaculatus, Notropis aetherinoides, Hyborhynchus notatus, Ambloplites rupestris, Huro salmonoides (Sax 1986).

MNO

1457 • 1-Naphthylamine 134-32-7

Synonyms	1-Aminonaphthalene	
Sumformula of the chemical	C10H9N	
Water solubility, mg/l	640	(MITI 1992)
Melting point, °C	50	(MITI 1992)
Boiling point, °C	300.8	(MITI 1992)
pKa	3.92	(Sangster 1989)
Log octanol/water coefficient, log Pow	2.25 2.25	(Sangster 1989) (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	13–54 9.1–27	8w, Cyprinus carpio, conc 0.2 mg/l 8w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	25	48hr, Oryzias latipes (MITI 1992)

1458 • 2-Naphthylamine sulfonic acid 81-16-3

Total degradation in water	Biodegradation: 3.8% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).	
Bioconcentration factor, fishes	< 0.6 < 6	8w, Cyprinus carpio, conc 5 mg/l 8w, Cyprinus carpio, conc 0.5 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	610	48hr, Oryzias latipes (MITI 1992)

1459 • 2-Naphthylisobutyl ether 2173-57-1

Sumformula of the chemical	C14H160	
Water solubility, mg/l	1.23	(MITI 1992)
Melting point, °C	31	(MITI 1992)
Log octanol/water coefficient, log Pow	5.24	(MITI 1992)

MNO

Total degradation in water	Biodegradation: 0–2% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	431–1180 398–873	8w, Cyprinus carpio, conc 0.05 mg/l 8w, Cyprinus carpio, conc 0.005 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	11.1	48hr, Oryzias latipes (MITI 1992)

1460 • Nickel and nickel compounds 7440-02-0

Molecular weight	58.71	
LDLo values to mammals in oral exposure, mg/kg	5	orl-gpg (Lewis & Sweet 1984)
Effects on plants	Soybean seeds (Glycine max) were planted in acid-washed sand. Beginning 5 days after seed germination the sand was saturated with metal solutions: Ni at 1 ppm caused reductions in stem and foliage dry weights (leaves and stems contained 0.00140 mg Ni/g (Vesper & Weidensaul 1978). Two cultivars of cotton (Gossypium spp.) were grown in solution culture. NiSO4 was phytotoxic at 0.00001 M (Rehab & Wallace 1978d).	
EC50 values to algae, mg/l	0.012 0.013	96hr, Selenastrum capricornutum 7d, Selenastrum capricornutum (Chiaudani & Vighi 1978)
LC50 values to crustaceans, mg/l	0.13 0.51 1.12	21d, Daphnia magna 48hr, without food, D.magna 48hr, with food, D.magna (Biesinger & Christensen 1972)
	119 435 66.1 252	Ni(II), mbt, 96hr, Asellus aquaticus Ni(II), mbt, 48hr, Asellus aquaticus Ni(II), mbt,96hr, Crangonyz pseudogracilis Ni(II), mbt,48hr, Crangonyz pseudogracilis (Martin & Holdich 1986)
	2000	Ni(II), 72hr, Asellus aquaticus (Braginskiy & Sherban 1978)
EC50 values to crustaceans, mg/l	7.5	48hr, mbt, Daphnia magna (Khangarot & Ray 1987)
	0.095	21d, rpd, Daphnia magna (Biesinger & Christensen 1972)
LOEC values to crustaceans, mg/l	0.03	21d, rpd, Daphnia magna (Biesinger & Christensen 1972)
LC50 values to fishes, mg/l	17.1	96hr, Salmo gairdneri (Anderson 1981)
	0.05	28d, S.gairdneri (Birge et al. 1980)
	307	96hr, Channa punctata (Saxena & Parashari 1983)
	13.6 24.5	96hr, Puntius gophore 96hr, Puntius gophore (Khangarot 1981)
	3.9 33 21	sfd, 96hr, Morone saxatilis, juv. hrd, 96hr, Morone saxatilis, juv. 1%., 96hr, Morone saxatilis, juv. (Palawski et al. 1985)
	35.5	96hr, Salmo gairdneri (Khangarot & Ray 1987)

LOEC values to fishes, mg/l	0.73	rpd, sch,hrd, Pimephales promelas (Pickering 1974)
NOEC values to fishes, mg/l	0.38	rpd, chr,hrd, Pimephales promelas (Pickering 1974)
Other information about water organisms	LC50 (96hr), 2.78 mg/l (Khangarot et al. 1982).	

1461 • Nickel chloride 7718-54-9

Synonyms	Nickelous chloride	
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 0.003 mg/l (Bringmann & Kühn 1980a).	
LC50 values to crustaceans, mg/l	10 7.3	1d, Daphnia magna 2d, Daphnia magna (Khangarot et al. 1987)
EC50 values to crustaceans, mg/l	10.9 7.59	mbt, 1d, Daphnia magna mbt, 2d, Daphnia magna (Khangarot & Ray 1987)
Effects on the physiology of water organisms	Nostoc muscorum, 1.0 mg/l, 0.02 d, photosynthesis effet (change in plant productivity indicated by change in 14C or CO2 uptake or oxygen consumption) (Rai & Raizada 1987).	
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 1.3 mg/l protozoa (Entosiphon sulcatum): 0.14 mg/l (Bringmann & Kühn 1980a)	

1462 • Nickel sulfate 7786-81-4

Synonyms	Nickelous sulfate	
Molecular weight	154.77	
LD50 values to mammals in non-oral exposure, mg/kg	21	ipr-mus (Lewis & Sweet 1984)
EC50 values to crustaceans, mg/l	435 119 252 66.1	mbt, 2d, Asellus aquaticus mbt, 4d, Asellus aquaticus mbt, 2d, Crangonyx pseudogracilis mbt, 4d, Crangonyx pseudogracilis (Martin & Holdich 1986)
LC50 values to fishes, mg/l	0.36 11.2 96.12 16.72	act, Salmo gairdneri (Russo et al. 1981) 14d, Oncorhynchus kisutch (Becker & Wolford 1980) 1d, Colisa fasciata 4d, Colisa fasciata (Kumar & Nath 1987)
EC50 values to fishes, mg/l	0.26	48hr, Salmo gairdneri (Anon. 1983)
LOEC values to fishes, mg/l	0.085	bhv, act, Salmo gairdneri (Anon. 1983)
Effects on the physiology of water organisms	Photosynthesis effect, 0.010 mg/l, 0.25 d, Anacystis nidulans; Spirulina platensis (Azeez & Banerjee 1987).	

MNO

1463 • Nicotine

54-11-5

Use	Active ingredient in insecticides.	
LD50 values to birds in oral exposure, mg/kg	17.8	orl-Agelaius phoeniceus
	42.2	orl-Sturnus vulgaris
	42.4–316	orl-Coturnix coturnix (Schafer et al. 1983)

1464 • Nicotine sulfate

65-30-5

Synonyms	3-(1-Methyl-2-pyrrolidine)pyridine sulfate 1-Methyl-2-(3-pyridyl)pyrrolidine sulfate Black leaf forty	
Sumformula of the chemical	C20H26N4.04S	
State and appearance	Solid or colourless solution. Will dissolve.	
Molecular weight	418.56	
Other physicochemical properties	Flammability: Moderate when exposed to heat or flame. Toxic combustion products: Sulfur compounds. Explosiveness: Moderate when exposed to heat or flame. Reactive at high temperature or pressure. Soluble.	
LD50 values to mammals in oral exposure, mg/kg	8.55	orl-mus
	83	orl-rat
	75	14d, orl-rat
	16	14d, orl-mus
	50	orl-rat (Sax 1986)
LD50 values to mammals in non-oral exposure, mg/kg	285	skn-rat
	29	ipr-rat (Sax 1986)
Health effects	Direct contact: irritant to skin. General sensation: Burning taste, develops pyridine odour. Causes nausea, vomiting, convulsions. Can be absorbed through skin. Acute hazard level: Irritant. Highly toxic via all routes. Emits toxic sulfur compounds when heated to decomposition. Chronic hazard level: Moderately toxic with chronic exposure via all routes (Sax 1986).	
Carcinogenicity	Rats fed nicotine for 6 months showed no tumors (Sax 1986).	
LD50 values to birds in oral exposure, mg/kg	75	orl-bwd (Sax 1986)
	75	orl-Agelaius phoeniceus
	> 100	orl-Sturnus vulgaris
	> 100	orl-Passer domesticus
	31.6–100	orl-Quiscalus quiscula
	75	orl-Columba livia
	100	orl-Carpodacus mexicanus
	75	orl-Anas platyrhynchos
	> 100	orl-Phasianus colchicus
	42.2	orl-Xanthocephalus xanthocephalus
	31.6	orl-Molothrus ater
	42.2	orl-Corvus brachyrhynchos
	56.2	orl-Zonotrichia leucophrys (Schafer et al. 1983)
Effects on arthropods	Tanytarsus dissimilis, LC50, > 27.0 mg/l, 2 d (Holcombe et al. 1987).	

MNO

LC50 values to crustaceans, mg/l	> 38.2	4d, Orconectes immunis (Holcombe et al. 1987)
EC50 values to crustaceans, mg/l	3.25	2d, mbt, Daphnia magna (Holcombe et al. 1987)
LC50 values to fishes, mg/l	13.1 4.31 19.7 7.31 12.2	4d, Carassius auratus 4d, Lepomis macrochirus 4d, Pimephales promelas 4d, Salmo gairdneri (Holcombe et al. 1987) 4d, Pimephales promelas (Geiger et al. 1988)
Other information about water organisms	Aplexa hypnorum, LC50, 4 d, > 38.2 mg/l (Holcombe et al. 1987). Fish, toxic effect, 3–29 mg/l, nicotine (Sax 1986).	
Other information	Air pollution high (Sax 1986).	

1465 • Nitric acid 7697-37-2

Synonyms	Hydrogen nitrate Nitryl hydroxide Azotic acid	
Sumformula of the chemical	HNO_3	
Purity, %	58.5–68 94.5–95.5	
Use	Medical, fertilizers, veterinary, dyes, explosives, chemicals.	
State and appearance	Corrosive colourless liquid. May get red brown tint in water.	
Odour	Acrid odour.	
Molecular weight	63.02	
Specific gravity (water=1)	1.502	
Vapour density (air=1)	3.2	
Vapour pressure, mmHg	42	20 °C
Melting point, °C	-41.6	
Boiling point, °C	86	
Other physicochemical properties	Solubility; miscible.	
Other information about degradation	Acid will slowly be neutralized, but nitrate can persist indefinitely (Sax 1986).	
LDLo values to mammals in oral exposure, mg/kg	430 110	orl-hmn unk-man (Sax 1986)
LDLo values to mammals in non-oral exposure, mg/kg	110	ukn-man (Sweet 1987)

LCLo values to mammals in inhalation exposure, ppm	244	NO2, ihl-rat, 30 min. NO2, ihl-rat. 4hr ihl-mus, 4hr
	65	NO2, ihl-rat, 30 min. NO2, ihl-rat. 4hr ihl-mus, 4hr
	67	NO2, ihl-rat, 30 min. NO2, ihl-rat. 4hr ihl-mus, 4hr (Sax 1986)
Health effects	Fumes are toxic. Ingestion causes burning of inner tissues, abdominal tenderness, shock, and death. Inhalation can cause chronic bronchitis or chemical pneumonitis. Chronic irritation is possible from prolonged contact. Nitrates are moderately toxic when chronically ingested or inhaled (Sax 1986).	
Effects on wastewater treatment	May upset pH enough to interfere with coagulation (Sax 1986).	
Other information about water organisms	Toxic: 1.6 mg/l, trout; 15.6 mg/l, 24hr, trout; 200 mg/l, minnows: 750 mg/l, 0.5hr, goldfish: 1000 mg/l, 0.5hr, trout; 1000 mg/l, 7hr, minnows (Sax 1986). Lethal: 750 mg/l, 0.5–0.8hr, goldfish (Sax 1986).	
Other information	Corrosive liquid; hazardous by all routes. Toxic to fish. NO3 is toxic to animal life even after neutralization. Emits toxic vapours when heated to decomposition (Sax 1986).	

1466 • Nitric acid, dodecyl ester 13277-59-3

Synonyms	Dodecyl nitrate Layryl nitrate
Sumformula of the chemical	C12H25NO3
Molecular weight	231.38
Other information about mammals	Skin and eye irritation data: skin, rabbit, 500 mg, 24hr, mild; eye, rabbit, 500 mg, 24hr, mild (Sweet 1987).

1467 • Nitriloacetic acid 139-13-9

LOEC values to algae, mg/l	8.3	rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
LC50 values to crustaceans, mg/l	> 100	act, Daphnia magna (Verschueren 1983)
LC50 values to fishes, mg/l	> 100	act, Pimephales promelas (Verschueren 1983)
	90.5	96hr, Salmo gairdneri
	92.3	96hr, Salmo gairdneri (Birge et al. 1979)

MNO

1468 • Nitrite ion

1594-56-5

Molecular weight	225.19	
LD50 values to mammals in oral exposure, mg/kg	2750	orl-mus (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	500	unk-mam (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	1650	orl-gpg (Lewis & Sweet 1984)
LC50 values to crustaceans, mg/l	28	96hr, Procambarus clarcii (Gutzmer & Tomasso 1985)
LC50 values to fishes, mg/l	0.3–12	96hr, Salmo gairdneri (Wedemayer & Yasutake 1978)
	0.6–31	96hr, Salmo gairdneri (Wedemayer & Yasutake 1978)
	13.7	96hr, Ictalurus punctatus (Tucker & Schwedler 1983)
	620	96hr, Branchydanio rerio
	135–565	48hr, Leuciscus idus (Wellens 1982)
	7.1	96hr, Ictalurus punctatus
	16.2	96hr, Sarotheredon aureus (Palachek & Tomasso 1984)
LOEC values to fishes, mg/l	0.45	phy, act, Salmo gairdneri (Arillo et al.1984)

1469 • 4-Nitro-1,2-diaminobenzene

99-56-9

Other information about water organisms	EC50 (60hr), 46 mg/l, rpd, Tetrahymena pyriformis (Schultz & Applehans 1985).

1470 • 5-Nitro-2-cresol

5428-54-6

Synonyms	5-Nitro-o-cresol	
Water solubility, mg/l	1000	(MITI 1992)
Melting point, °C	118	(MITI 1992)
Log octanol/water coefficient, log Pow	2.47	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	4.2–10	6w, Cyprinus carpio, conc 0.3 mg/l
	< 4.3–6.9	6w, Cyprinus carpio, conc 0.03 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	16.3	48hr, Oryzias latipes (MITI 1992)

MNO

1471 • 4-Nitro-m-cresol 2581-34-2

Water solubility, mg/l	1000 (MITI 1992)
Melting point, °C	129 (MITI 1992)
Log octanol/water coefficient, log Pow	2.12 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	5.2–31 6w, Cyprinus carpio, conc 0.3 mg/l 6.0–17 6w, Cyprinus carpio, conc 0.03 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987) (4-nitro-3-cresol).
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 6 mg/l (Bringmann & Kühn 1980a).
LC50 values to fishes, mg/l	16 48hr, Oryzias latipes (MITI 1992)
Other information about water organisms	LOEC 0.26 mg/l, rpd, schr, Uronema parduczi (Bringmann & Kühn 1980b). LOEC 5.8 mg/l, rpd, schr, Entosiphon sulcatum (Bringmann & Kühn 1980a). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 6.8 mg/l protozoa (Entosiphon sulcatum): 5.8 mg/l (Bringmann & Kühn 1980a)

1472 • 4-Nitro-o-anisidine 85-45-0

Sumformula of the chemical	C7H8N2O3
EINECS-number	2016080
Water solubility, mg/l	< 100 (MITI 1992)
Melting point, °C	138.9–141.2 (MITI 1992)
Log octanol/water coefficient, log Pow	1.78 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

1473 • 2-Nitro-p-anisidine 96-96-8

Sumformula of the chemical	C7H8N2O3
EINECS-number	2025472
Water solubility, mg/l	120 (MITI 1992)
Melting point, °C	12–125 (MITI 1992)

Log octanol/water coefficient, log Pow	1.94 (MITI 1992)
Total degradation in water	Biodegradation: 0–4% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992)
Bioconcentration factor, fishes	2.8–4.6 6w, Cyprinus carpio, conc 0.25 mg/l < 6.2–7.0 6w, Cyprinus carpio, conc 0.025 mg/l (MITI 1992)
LC50 values to fishes, mg/l	41.1 48hr, Oryzias latipes (MITI 1992)

1474 • 2-Nitro-p-cresol 119-33-5

Synonyms	2-Nitro-4-cresol
Water solubility, mg/l	633 (MITI 1992)
Melting point, °C	36.5 (MITI 1992)
Boiling point, °C	125 22 mmHg (MITI 1992)
Log octanol/water coefficient, log Pow	2.37 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	4.2–9.1 6w, Cyprinus carpio, conc 0.3 mg/l < 5.0–13 6w, Cyprinus carpio, conc 0.03 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987) (2-nitro-4-cresol).
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 4 mg/l (Bringmann & Kühn 1980a).
LOEC values to algae, mg/l	3.8 rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
LC50 values to fishes, mg/l	70 (MITI 1992)
Other information about water organisms	LOEC 0.42 mg/l, rpd, schr, Entosiphon sulcatum (Bringmann & Kühn 1980a). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 3.8 mg/l protozoa (Entosiphon sulcatum): 0.42 mg/l (Bringmann & Kühn 1980a)

1475 • 3-Nitro-p-cresol 2042-14-0

Synonyms	4-Methyl-3-nitrophenol
Sumformula of the chemical	C7H7N03
EINECS-number	2180446
Water solubility, mg/l	> 1000 (MITI 1992)

MNO

Melting point, °C	79	(MITI 1992)
Log octanol/water coefficient, log Pow	2.18	(MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon.1987).	
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	4.0–12 6.1–14	6w, Cyprinus carpio, conc 0.3 mg/l 6w, Cyprinus carpio, conc 0.03 mg/l (MITI 1992)
LC50 values to fishes, mg/l	20.4	48hr, Oryzias latipes (MITI 1992)

1476 • 2-Nitroaniline

88-74-4

Water solubility, mg/l	0.12	(MITI 1992)
Melting point, °C	72.5–73.5	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).	
Bioconcentration factor, fishes	2.1–4.9 < 10	6w, Cyprinus carpio, conc 0.5 mg/l 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LD50 values to birds in oral exposure, mg/kg	750 ≥ 1000 750 750	orl-Agelaius phoeniceus orl-Sturnus vulgaris orl-Coturnix coturnix orl-Passer-domesticus (Schafer et al. 1983)
LC50 values to fishes, mg/l	17	48hr, Oryzias latipes (MITI 1992)
Other information about water organisms	EC50 (60hr), 116 mg/l, rpd, Tetrahymena pyriformis (Schultz & Applehans 1985).	

1477 • 3-Nitroaniline

99-09-2

Melting point, °C	114	(MITI 1992)
Boiling point, °C	> 285	(MITI 1992)

Total degradation in water	Biodegradaation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Bioconcentration factor, fishes	1.1–3.0 6w, Cyprinus carpio, conc 0.5 mg/l < 10 6w, Cyprinus carpio, conc 0.5 mg/ (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to birds in oral exposure, mg/kg	133 orl-Agelaius phoeniceus > 1000 orl-Sturnus vulgaris 562 orl-Coturnix coturnix > 1000 orl-Passer domesticus (Schafer et al. 1983)
LC50 values to fishes, mg/l	96 48hr, Oryzias latipes (MITI 1992)

1478 • 4-Nitroaniline

100-01-6

Synonyms	1-Amino-4-nitrobenzene p-Nitroaniline 4-Aminonitrobenzene
Sumformula of the chemical	C6H6N2O2
Use	Intermediate for dyes and antioxidants, gasoline gum inhibitors, medicinals for poultry, corrosion inhibitor.
State and appearance	Yellow monoclinic needles.
Molecular weight	138.14
Vapour pressure, mmHg	0.0015 20 °C
Water solubility, mg/l	800 19 °C
Melting point, °C	148.5–150 (MITI 1992)
Boiling point, °C	260–332, decomposes
Log octanol/water coefficient, log Pow	2.66 (Anon. 1988)
Log soil sorption coefficient, log Kom	1.64 (Sabljic 1987)
Henry's law constant, Pa x m³/mol	0.035 (Anon. 1988)
Mobility	Equilibrium distribution: *mass %* air 1.10 water 92.42 solid 6.49 (Anon. 1988).
Total degradation in soil	Biodegradation: decomposition by a soil micro flora in > 64 days (Verschueren 1983).

MNO

Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Bioconcentration factor, fishes	2.9–3.6 6w, Cyprinus caarpio, conc 0.5 mg/l < 10 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	750 orl-rat 450 orl-gpg (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	75 orl-bwd (Lewis & Sweet 1984) 75.0–100 orl-Agelaius phoeniceus > 1000 orl-Sturnus vulgaris 1000 orl-Coturnix coturnix (Schafer et al. 1983)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 4 mg/l (Bringmann & Kühn 1980a)
LOEC values to algae, mg/l	0.35 rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to fishes, mg/l	35 48hr, Leuciscus idus 87.6 96hr, Branchydanio rerio (Wellens 1982) 106 96hr, Pimephales promelas (Curtis & Ward 1981) 84 48hr, Oryzias latipes (MITI 1992)
Other information about water organisms	LOEC 3.1 mg/l, rpd, schr, Uronema parduczi (Bringmann & Kühn 1980b). EC50 (60hr), 10 mg/l, rpd, Tetrahymena pyriformis (Schultz & Applehans 1985). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 11 mg/l protozoa (Entosiphon sulcatum): 6.9 mg/l (Bringmann & Kühn 1980a).

1479 • 2-Nitroanisole

91-23-6

Synonyms	o-Nitroanisole
Melting point, °C	10 (MITI 1992)
Boiling point, °C	265 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).

Bioconcentration factor, fishes	1.4–2.3 8w, Cyprinus carpio, conc 0.05 mg/l 2.7–5.2 8w, Cyprinus carpio, conc 0.005 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	25 48hr, Oryzias latipes (MITI 1992)

1480 • 4-Nitroanisole 100-17-4

Synonyms	1-Methoxy-4-nitrobenzene 4-Nitrophenylmethyl ether p-Methoxynitrobenzene
Sumformula of the chemical	C7H7NO3
EINECS-number	2028253
Water solubility, mg/l	600 (MITI 1992)
Melting point, °C	54 (MITI 1992)
Boiling point, °C	259 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Bioconcentration factor, fishes	0.8–3.0 6w, Cyprinus carpio, conc 0.05 mg/l < 6–18.6 6w, Cyprinus carpio, conc 0.005 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	55 48hr, Oryzias latipes (MITI 1992)

MNO

1481 • Nitrobenzene 98-95-3

Sumformula of the chemical	C6H5NO2
Use	Manufacturing aniline and dyestuffs; solvent recovery plants; solvent in TNT production; intermediate (99,9%).
State and appearance	Yellow liquid.
Molecular weight	123.12
Vapour pressure, mmHg	0.15 20 °C
Water solubility, mg/l	1900 20 °C (Anon. 1986b)
Melting point, °C	5.85 (MITI 1992)
Boiling point, °C	210 (Anon. 1986b) 210.85 (MITI 1992)

Log octanol/water coefficient, log Pow	1.85 (Anon. 1986) 1.89 (Chin et al. 1986) 1.84 (Anon. 1986b) 2.15 (Anon. 1988) 2.93 (Mackay 1982) 1.84 (Sangster 1989)
Log soil sorption coefficient, log Kom	1.7 (Sabljic 1987)
Henry's law constant, Pa x m³/mol	1.3 (Anon. 1988)
Volatilization	Relative volatility (nBuAc=1) = 0.026
Mobility	Equilibrium distribution: *mass %* air 30.49 water 68.04 solid 1.47 (Anon. 1988).
Total degradation in soil	Biodegradation: decomposition by a soil microflora in > 64 days (Verschueren 1983).
Total degradation in water	Biodegradation: 3.3% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992)
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Bioconcentration factor, fishes	3.1–4.8 6w, Cyprinus carpio, conc 0.125 mg/l 1.6–7.7 6w, Cyprinus carpio, conc 0.0125 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	640 orl-rat 59 orl-mus (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	2100 skn-rat (Lewis & Sweet 1984)
LDLo values to mammals in oral exposure, mg/kg	750 orl-dog (Anon. 1986b) 2000 orl-cat (Anon. 1986b) 700 orl-rbt (Anon. 1986b)
LDLo values to mammals in non-oral exposure, mg/kg	35 unk-man 600 skn-rbt (Lewis & Sweet 1984)
Maximum longterm immission concentration in air for plants, mg/m³	0.3 VDI 2306
Maximum longterm immission concentration in air for plants, ppm	0.05 VDI 2306
Effects on microorganisms	EC50, Photobacterium phosphoreum, 46.2 mg/l, 5 min (Anon. 1986b) Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 7 mg/l (Bringmann & Kühn 1980a)

EC50 values to microorganism, mg/l	28	Microtox (Kaiser and Ribo 1985)
EC50 values to algae, mg/l	44.1 42.8	96hr, Selenastrum capricornutum chlorophyll a (Anon. 1986b) 96hr, Selenastrum capricornutum cellnumber (Anon. 1986b)
LOEC values to algae, mg/l	1.9	rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to crustaceans, mg/l	27	48hr, Daphnia magna (LeBlanc 1980)
	27 62 34	48hr, Daphnia magna 2d, Daphnia magna 21d, Daphnia magna (Anon. 1986b)
EC50 values to crustaceans, mg/l	12	rpd, 14 d, Daphnia magna (Hattori et al. 1984)
	50 60 35	24hr, Daphnia magna 24hr, Daphnia magna 2d, Daphnia magna (Anon. 1986b)
LC50 values to fishes, mg/l	0.002	96hr, Salmo gairdneri (juv.) (Black et al. 1982)
	0.6–7.0	96hr, Pimephales promelas (Bailey & Spanggord 1983)
	112.5 60–89	96hr, Branchydanio rerio 48hr, Leuciscus idus (Wellens 1982)
	43	96hr, Lepomis macrochirus (Buccafusco et al. 1981)
	59	96hr, Cyprinodon variegatus (Heitmüller et al. 1981)
	60/89 42.6 24	mg/l, 48hr, Leuciscus idus 96hr, Lepomis macrochirus 40d, Oryzias latipes (Anon. 1986b)
	117	96hr, Pimephales promelas (Holcombe et al. 1983)
	125	48hr, Oryzias latipes (MITI 1992)
EC50 values to fishes, mg/l	32 23	empryo-larvae-test, Pimephales promelas (Anon. 1986b) 40d, srv, Oryzias latipes (Anon. 1986b)
NOEC values to fishes, mg/l	7.6	40d, srv, Oryzias latipes (Anon. 1986b)
Other information about water organisms	EC50 (24hr), 98 mg/l, rpd, Tetrahymena pyriformis (Yoshioka et al. 1985). LOEC 1.9 mg/l, rps, schr, Entosiphon sulcatum (Bringmann & Kühn 1980a). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 33 mg/l protozoa (Entosiphon sulcatum): 1.9 mg/l (Bringmann & Kühn 1980a)	

1482 • 5-Nitrobenzimidazole 94-52-0

Water solubility, mg/l	> 250	(MITI 1992)
Melting point, °C	204	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

Bioconcentration factor, fishes	0.7–1.8 < 2.9	6w, Cyprinus carpio, conc 0.5 mg/l 6w, Cyprinus carpio, 0.05 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	27.8	48hr, Oryzias latipes (MITI 1992)

1483 • 2-Nitrobenzoic acid 552-16-9

Synonyms	o-Nitrobenzoic acid	
Water solubility, mg/l	100	(MITI 1992)
Melting point, °C	146–148	(MITI 1992)
Total degradation in water	Biodegradation: 100% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	

1484 • 3-Nitrobenzoic acid 121-92-6

Synonyms	m-Nitrobenzoic acid	
Water solubility, mg/l	100	(MITI 1992)
Melting point, °C	140–141	(MITI 1992)
Log octanol/water coefficient, log Pow	1.83	(Anon. 1986)
Total degradation in water	Biodegradation: 0-12% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.7 < 7.1	6w, Cyprinus carpio, conc 0.3 mg/l 6w, Cyprinus carpio, conc 0.03 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	> 50	48hr, Oryzias latipes (MITI 1992)

1485 • 4-Nitrobenzoic acid 62-23-7

Water solubility, mg/l	100	(MITI 1992)
Melting point, °C	238	(MITI 1992)

Total degradation in water	Biodegradation: 62% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	

1486 • 3-Nitrobenzonitrile 619-24-9

EC50 values to crustaceans, mg/l	48.1	mbt, 48hr, Daphnia magna (Pearson et al. 1979)
LC50 values to fishes, mg/l	60.2	96hr, Pimephales promelas (Pearson et al. 1979)

1487 • 4-Nitrobenzonitrile 619-72-7

EC50 values to crustaceans, mg/l	49.4	mbt, 48hr, Daphnia magna (Pearson et al. 1979)
LC50 values to fishes, mg/l	24.4	96hr, Pimephales promelas (Pearson et al. 1979)

1488 • 5-Nitrobenzotriazole 2338-12-7

Other information about water organisms	EC50 (60hr), 29 mg/l, rpd, Tetrahymena pyriformis (Schultz & Applehans 1985).

1489 • Nitroethane 79-24-3

Sumformula of the chemical	C2H5NO2	
Use	Solvent.	
Water solubility, mg/l	45000	20 °C
Boiling point, °C	114–115	
Log octanol/water coefficient, log Pow	0.18	(Sangster 1989)
Volatilization	Relative volatility (nBuAc=1) = 1.03	
LD50 values to mammals in oral exposure, mg/kg	1100	orl-rat

1490 • Nitrofurazone 59-87-0

EC50 values to algae, mg/l	1.45	96hr, rpd, Selenastrum capricornutum (Macri & Sbardella 1984)
EC50 values to crustaceans, mg/l	40 29	24hr, srv, Daphnia magna 48hr, srv, Daphnia magna (Macri & Sbardella 1984)

MNO

1491 • Nitrogen dioxide 10102-44-0

Effects on plants	Controlled levels of pollutants were added for 103.5 h weakly, clean air being given for the remaining 64.5 h. The concentration of each gas used during 103.5 h exposure was 0.11 ppm. The treatments with concentrations calculated as weekly means were (as follows) 0.068 ppm → yields of Dactylis glomerata and Poa pratensis were reduced (Ashenden & Mansfield 1978).

1492 • 5-Nitroindole 6146-52-7

Other information about water organisms	EC50 (60hr), 13 mg/l, rpd, Tetrahymena pyriformis (Schultz & Applehans 1985).

1493 • 5-Nitrokinoline 607-34-1

Other information about water organisms	EC50 (60hr), 71 mg/l, rpd, Tetrahymena pyriformis (Schultz & (Applehans 1985)).

1494 • 6-Nitrokinoline 613-50-3

Effects on water organisms	EC50 (60hr), 60 mg/l, rpd, Tetrahymena pyriformis (Schultz & Applehans 1985).

1495 • Nitromethane 75-52-5

Sumformula of the chemical	CH3NO2	
Use	Solvent.	
Water solubility, mg/l	98000	20 °C
Boiling point, °C	101.2	
Log octanol/water coefficient, log Pow	-0.33	(Sangster 1989)
Henry's law constant, Pa x m³/mol	27.48	calc. (Yaws et al. 1991)
Volatilization	Relative volatility (nBuAc=1) = 1.27	
LD50 values to mammals in oral exposure, mg/kg	940	orl-rat

1496 • 1-Nitronaphthalene 86-57-7

LC50 values to fishes, mg/l	9	96hr, Pimephales promelas (Curtis & Ward 1981)

1497 • 2-Nitrophenol 88-75-5

Synonyms	o-Nitrophenol 2-Hydroxynitrobenzene o-Hydroxynitrobenzene
Sumformula of the chemical	C6H5NO3
Use	Indicator; intermediate in organic synthesis; fungicide for leather.

State and appearance	Light yellow needles will sink, and quick action could recover most of the material from the bottom before it dissolves.
Molecular weight	139.11
Specific gravity (water=1)	1.49
Vapour pressure, mmHg	1 49.3 °C
Water solubility, mg/l	2100 20 °C 10000 100 °C > 100 (MITI 1992)
Melting point, °C	44.6 (MITI 1992)
Boiling point, °C	216 (MITI 1992)
Flashing point, °C	73.5
Log octanol/water coefficient, log Pow	1.75 (Anon. 1986)
Other physicochemical properties	Flammability: combustible solid. Toxic combustion products: highly toxic NOx are emitted. Odour and taste problems are accented by chlorination of the contaminated water. Will give acid solution.

Aerobic degradation in water

Biochemical oxygen demand:

Lb/Lb	*%Theo*	*Days*	*Seed*	*Method*
2.16	90	5	sewage	standard method for phenol
2.136	89	10	sewage	standard method for phenol
2.088	87	15	sewage	standard method for phenol
2.304	96	20	sewage	standard method for phenol

(Sax 1986).

Total degradation in water

Biodegradation:
0% by BOD
period: 28d
substance: 30 mg/l
sludge: 100 mg/l
(MITI 1992).

Other information about degradation

Degradation of 2-nitrophenol:

ENVIRONMENT	*INIT.CONC. mg/l*	*REDOX-COND.*	*TEMP. °C*	*DEGRADATION % /day*	*REF.*
water	5	aerobic	25	100/7	a
water	10	aerobic	25	100/7	a
water	20	aerobic	25	81/7	b
water (adapted)	20	aerobic	25	99/28	b
waste water	16	aerobic	30	100/3-5	c
soil	16	aerobic	30	100/7-14	c
soil suspension	15	aerobic	25	< 100/64	d
soil	30	aerobic	28	63/10	e
soil (adapted+)	30	aerobic	28	95/10	e
soil	29	aerobic	28	50/10	e
soil (adapted+)	29	aerobic	28	77/10	e

+ adapted to parathion

a) Tabak et al. 1981 b) Bunch & Chamber 1967
c) Haller 1978 d) Alexander & Lustigman 1966
e) Sudhakar-Barik et al. 1979 (Anon. 1987b).

Persistent; o-nitrophenol resisted degradation in the soil bacillus bacterium (Sax 1986).

Bioconcentration factor, fishes	< 2.2–5.0 6w, Cyprinus carpio, conc 1 mg/l < 22 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987). Nitrophenols are not expected to be accumulated in the food chain (Sax 1986).
LD50 values to mammals in oral exposure, mg/kg	2828 orl-rat 1297 orl-rat 1300 orl-mus (Sax 1986)
LDLo values to mammals in non-oral exposure, mg/kg	100 ivn-dog 1100 scu-dog 600 scu-cat 1700 scu-rbt 900 scu-gpg (Sax 1986)
Health effects	Direct contact: Contact with eyes causes irritation. Absorbed via intact skin to give same symptoms as for inhalation. General sensation: Inhalation or ingestion causes headache, drowsiness, nausea, and cyanosis. Irritant to eyes and skin. If material contacts skin, wash immediately and seek medical aid at once (Sax 1986).
Carcinogenicity	Nitrophenols are suspected cocarcinogens with polycyclic hydrocarbons when applied to mouse skins (Sax 1986).
Effects on amphibia	LDLo, 300 mg/kg, scu, frog (Sax 1986).
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 0.9 mg/l (Bringmann & Kühn 1980a)
Effects on wastewater treatment	Use 10 to 35 lb. of carbon per lb. of material. Additional treatment will be necessary to alleviate the phenolic taste in water. The chlorinated phenols present problems in drinking water supplies because phenol is not removed efficiently by conventional water treatment and can be chlorinated during the final water treatment process to form persistent odour-producing compounds (Sax 1986).
LC50 values to fishes, mg/l	46 96hr, Lepomis macrochirus (Jones 1971) 160 96hr, Pimephales promelas (Geiger et al. 1988) 100 48hr, Oryzias latipes (MITI 1992)
Other information about water organisms	EC50 (24hr), 35 mg/l, rpd, Tetrahymena pyriformis (Yoshioka et al. 1985). LOEC 0.4 mg/l, rpd, schr, Entosiphon sulcatum (Bringmann & Kühn 1980a). Mild effect, minnows, 22 °C, 6hr: 14–18 mg/l, distilled; 125–130 mg/l, hard (Sax 1986). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 4.3 mg/l protozoa (Entosiphon sulcatum): 0.4 mg/l (Bringmann & Kühn 1980a)
Other information	Air pollution: Highly toxic NOx and fumes of unburned material may form in fires (Sax 1986).

1498 • 3-Nitrophenol 554-84-7

Synonyms	m-Nitrophenol
Melting point, °C	97 (MITI 1992)
Boiling point, °C	194 70 mmHg (MITI 1992)

MNO

Total degradation in water	Biodegradation: 48% by BOD period: 14d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
Other information about degradation	Degradation of 3-nitrophenol:

ENVIRONMENT	*INIT.CONC. mg/l*	*REDOX-COND.*	*TEMP. °C*	*DEGRADATION %/day*	*REF.*
sludge	200	aerobic	–	20/10	a
sludge	200	aerobic	–	50/12	a
sludge	200	aerobic	–	90/16	a
sludge (adapted)	200	aerobic	–	20/1	a
sludge (adapted)	200	aerobic	–	50/2	a
sludge (adapted)	200	aerobic	–	90/6	a
waste water	16	aerobic	30	100/3-5	b
soil	16	aerobic	30	100/3-5	b
soil suspension	10	aerobic	25	100/4	c
soil	25	aerobic	28	72/10	d
soil (adapted+)	25	aerobic	28	100/10	d
soil	24	aerobic	28	68/10	d
soil (adapted+)	24	aerobic	28	92/10	d

+ adapted to parathion

a) Zahn & Wellens 1980 b) Haller 1978
c) Alexander & Lustigman 1966 d) Sundhakar-Barik et al. 1979
(Anon. 1987b).

Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 7 mg/l (Bringmann & Kühn 1980a).
Other information about water organisms	EC50 (24hr), 28 mg/l, rpd, Tetrahymena pyriformis (Yoshioka et al. 1985). LOEC 0.97 mg/l, rpd, schr, Entosiphon sulcatum (Bringmann & Kühn 1980a). LOEC 3.4 mg/l, rpd, schr, Uronema parduczi (Bringmann & Kühn 1980b). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 7.6 mg/l protozoa (Entosiphon sulcatum): 0.97 mg/l (Bringmann & Kühn 1980a).

MNO

1499 • 4-Nitrophenol 100-02-7

Synonyms	p-Nitrophenol	
Use	Intermediate in organic synthesis; production of parathion; fungicide for leather.	
State and appearance	Colourless to yellowish crystals.	
Molecular weight	139.12	
Vapour pressure, mmHg	2.2	146 °C
Water solubility, mg/l	16000	25 °C
Melting point, °C	114.6	(MITI 1992)
Boiling point, °C	279	(MITI 1992)
Degradation point, °C	279	

Log octanol/water coefficient, log Pow	2.91 (Mackay 1982)
Total degradation in soil	Biodegradation: decomposition by soil microflora in 16 days (Verschueren 1983). Biodegradation: 4.3% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Other information about degradation	Degradation of 4-nitrophenol:

ENVIRONMENT	*INIT.CONC. mg/l*	*REDOX-COND.*	*TEMP. °C*	*DEGRADATION %/day*	*REF.*
water	5	aerobic	25	100/7	a
water	10	aerobic	25	100/7	a
water	100	aerobic	22	5/25	b
water	100	aerobic	22	0/25	b
water	100	aerobic	22	0/25	b
sediment	100	aerobic	22	25/25	b
sediment	100	aerobic	22	0/25	b
sediment	100	aerobic	22	100/25	b
lake water	0.0002	aerobic	29	72/26	c
lake water	5	aerobic	21	80-95/11	d
slugde	40	aerobic	22	100/1-3	e
slugde	100	aerobic	22	100/1-4	e
slugde	400	aerobic	22	100/5	e
slugde	800	aerobic	22	100/6	e
slugde	100	anaerobic	35	91/14	f
slugde	100	anaerobic	35	99/14	f
waste water	16	aerobic	30	100/3-5	f
soil	16	aerobic	30	100/7-14	g
soil suspension	5	aerobic	25	100/16	h
soil	–	aerobic	20	100/5	i
soil	19	aerobic	–	80/28	k
soil	2	aerobic	10	> 90/4	l
soil	2	anaerobic	10	> 90/60	l
soil	0.5	aerobic	21	31/2.5	m
soil	5	aerobic	21	33/2.5	m
soil	50	aerobic	21	18/2.5	m
soil	22	aerobic	28	51/10	n
soil (adapted+)	27	aerobic	28	100/5	n
soil	35	aerobic	28	70/10	n
soil (adapted+)	32	aerobic	28	80/10	n

+ adapted to parathion

a) Tabak et al. 1981
b) Van Veld & Spain 1983
c) Subba-rao et al. 1982
d) Goldstein et al. 1985
e) Nyholm et al. 1984
f) Horowitz et al. 1982
g) Haller 1978
h) Alexander & Lustigman 1966
i) Lindegaard-Jörgensen 1983
k) Kool 1984
l) Lökke 1985
m) Scow et al. 1986
n) Sudhakar-Barik et al. 1979
(Anon. 1987b).

Bioconcentration factor, fishes	2.5–7.8 6w, Cyprinus carpio, conc 0.2 mg/l 2.6–5.4 6w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)

MNO

Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	250 247	orl-rat orl-mam (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	150 920	unk-cat skn-mam (Lewis & Sweet 1984)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 4 mg/l (Bringmann & Kühn 1980a)	
EC50 values to microorganism, mg/l	63–130 126	3hr Act. sludge respiration (King and Painter 1986) OECD 209 (Klecka et al. 1985)
EC50 values to algae, mg/l	32	96hr, grw, Scenedesmus subspicatus (Geyer et al. 1985)
LC50 values to crustaceans, mg/l	22	48hr, Daphnia magna, LeBlanc 1980
LC50 values to fishes, mg/l	8.3	96hr, Lepomis macrochirus (Buccafusco et al. 1981)
	27	96hr, Cyprinodon variegatus (Heitmuller et al. 1981)
	10	48hr, Pimephales promelas (Phipps et al. 1981)
	41 15	96hr, Pimephales promelas 96hr, Ictalurus punctatus (Holcombe et al. 1984)
	7.9	act, Salmo gairdneri (Hodson et al. 1984)
	19.8	48hr, Oryzias latipes (MITI 1992)
LOEC values to fishes, mg/l	16	srv, schr, Cypronodon variegatus (Ward & Parrish 1980)
Other information about water organisms	EC50 (24hr), 5.5 mg/l, rpd, Tetrahymena pyriformis (Yoshioka et al. 1985). LOEC 0.83 mg/l, rpd, schr, Entosiphon sulcatum (Bringmann & Kühn 1980a). LOEC 0.89 mg/l, rpd, schr, Uronema parduczi (Bringmann & Kühn 1980b). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 7.4 mg/l protozoa (Entosiphon sulcatum): 0.83 mg/l (Bringmann & Kühn 1980a)	

1500 • p-Nitrophenyl phenylether 620-88-2

Synonyms	p-Nitrodiphenyl ether	
LD50 values to birds in oral exposure, mg/kg	> 100	orl-Agelaius pheoniceus (Schafer et al. 1983)
LC50 values to fishes, mg/l	2.7	96hr, Pimephales promelas (Veith et al. 1983)

1501 • 3-Nitrophthalic acid 603-11-2

Water solubility, mg/l	1000	(MITI 1992)
Melting point, °C	218	(MITI 1992)
Log octanol/water coefficient, log Pow	-0.93	(MITI 1992)

Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.4 6w, Cyprinus carpio, conc 1 mg/l < 3.9–6.5 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	260 48hr, Oryzias latipes (MITI 1992)

1502 • 1-Nitropropane 108-03-2

Sumformula of the chemical	C3H7NO2
Use	Solvent.
Water solubility, mg/l	14000 20 °C
Boiling point, °C	131.6
Log octanol/water coefficient, log Pow	0.87 (Sangster 1989)
Henry's law constant, Pa x m³/mol	6.399 calc. (Yaws et al. 1991)
Volatilization	Relative volatility (nBuAc=1) = 0.79
LD50 values to mammals in oral exposure, mg/kg	800 orl-mus

1503 • 2-Nitropropane 79-46-9

Use	Solvent.
Water solubility, mg/l	12000 (MITI 1992)
Boiling point, °C	120.3 (MITI 1992)
Log octanol/water coefficient, log Pow	0.93 (MITI 1992)
Henry's law constant, Pa x m³/mol	9.048 calc (Yaws et al. 1991)
Volatilization	Relative volatility (nBuAc=1) = 1.04
Total degradation in water	Biodegradation: 14% by BOD 8% by BOD period: 28d period: 28d substance: 2.0 mg/l substance: 9.9 mg/l sludge: 2mg/l sludge 2 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.9–1.1 6w, Cyprinus carpio, conc 2 mg/l < 8.4 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
LDLo values to mammals in oral exposure, mg/kg	500 orl-rat
LC50 values to fishes, mg/l	808 48hr, Oryzias latipes (MITI 1992)

MNO

1504 • 4-Nitropyridine 1122-61-8

Other information about water organisms	EC50 (60hr), 48 mg/l, rpd, Tetrahymena pyriformis (Schultz & Applehans 1985).

1505 • n-Nitrosodiethylamine 55-18-5

LC50 values to fishes, mg/l	775	96hr, Pimephales promelas (Draper & Brewer 1979)

1506 • n-Nitrosodiphenylamine 86-30-6

Melting point, °C	64–66 (MITI 1992)	
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	8.1–42 4.6–38	6w, Cyprinus carpio, conc 0.2 mg/l 6w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to crustaceans, mg/l	7.8	48hr, Daphnia magna (LeBlanc 1980)
LC50 values to fishes, mg/l	6.4	48hr, Oryzias latipes (MITI 1992)

1507 • β-Nitrostyrene 102-96-5

Other information about mammals	LDfr = 12.5 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

MNO

1508 • m-Nitrotoluene 99-08-1

Synonyms	m-Methylnitrobenzene 3-Methylnitrobenzene 3-Nitrotoluene 3-Nitrotoluol	
Sumformula of the chemical	C7H7NO2	
Molecular weight	137.15	
Water solubility, mg/l	440 300	30 °C (Anon. 1986b) (MITI 1992)
Melting point, °C	16	(MITI 1992)
Boiling point, °C	232.6 227.2–227.5	(Anon. 1986b) (MITI 1992)
Log octanol/water coefficient, log Pow	2.45 2.45 2.4	(Anon. 1986b) (Sangster 1989) (MITI 1992)

Total degradation in water	Biodegradation: 2% by BOD period: 14w substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	28 Salmon, mussel/water (Anon. 1986b) 0.47–8.5 06w, Cyprinus carpio, conc 0.025 mg/l 3–12 6w, Cyprinus carpio, conc 0.0025 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	3600 orl-gpg 330 orl-mus 1072 orl-rbt (Sweet 1987)
Effects on amphibia	LC50, Xaenopus laevis, 9,0 mg/l, 4d (Anon. 1986b) EC50, Xaenopus laevis, 2,5 mg/l, 4d (Anon. 1986b)
Effects on arthropods	LC50, Culex pripiens, 30 mg/l, 2d (Anon. 1986b)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 10 mg/l (Bringmann & Kühn 1980a)
LOEC values to algae, mg/l	4.4 rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a) 1 rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to crustaceans, mg/l	17.6 2d, Daphnia magna (Anon. 1986b) 9 21d, Daphnia magna (Anon. 1986b)
EC50 values to crustaceans, mg/l	24 24hr, Daphnia magna (Anon. 1986b) 7.4 2d, Daphnia magna (Anon. 1986b) 9 21d, srv, Daphnia magna (Anon. 1986b) 3.5 21d, rpd, Daphnia magna (Anon. 1986b)
NOEC values to crustaceans, mg/l	0.5 21d, Daphnia magna (Anon. 1986b)
LC50 values to fishes, mg/l	30 96hr, Pimephales promelas (Vincent et al. 1976) 37 4d, Poecilia reticulate 30 4d, Oryzias latipes 9.9 40d, Oryzias latipes (Anon. 1986b) 71 48hr, Oryzias latipes (MITI 1992)
EC50 values to fishes, mg/l	7.4 4d, Poecilia reticulate 4.1 40d, Oryzias latipes 3 40d, srv, Oryzias latipes (Anon. 1986b)
NOEC values to fishes, mg/l	2 40d, rpd, Oryzias latipes (Anon. 1986b)
Other information about water organisms	EC50 (24hr), 50 mg/l, rpd, Tetrahymena pyriformis (Yoshioka et al. 1985). LC50, Lymnaea stagnalis, 20 mg/l, 4d (Anon. 1986b) Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 4.4 mg/l protozoa (Entosiphon sulcatum): 12 mg/l (Bringmann & Kühn 1980a)

MNO

1509 • o-Nitrotoluene 88-72-2

Synonyms	o-Methylnitrobenzene 2-Nitrotoluene 1-Methyl-2-nitrobenzene 2-Methyl-1-nitrobenzene 2-Methylnitrobenzene	
Sumformula of the chemical	C7H7NO2	
Purity, %	> 99% (w/v)	
Known impurities	1-methyl-3-nitrobenzene1-methyl-4-nitrobenzene	
Vapour pressure, mmHg	1	at 50 °C
Water solubility, mg/l	540	at 20 °C (Meskens 1990)
Melting point, °C	-3.4	(MITI 1992)
Boiling point, °C	225 221.7	(Meskens 1990) (MITI 1992)
Log octanol/water coefficient, log Pow	2.3	(Sangster 1989)
Total degradation in water	Biodegradation: 0.5% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).	
Bioconcentration factor, fishes	12.5–29.9 6.6–29.7	6w, Cyprinus carpio, conc 0.1 mg/l 6w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 18 mg/l (Bringmann & Kühn 1980a)	
LOEC values to algae, mg/l	3.1	rpd, schr, Microcystis aueruginosa (Bringmann & Kühn 1976)
LC50 values to crustaceans, mg/l	> 77.1 8.8	mg/l, 48hr, Daphnia magna (Liu et al. 1983) 48hr, Daphnia magna (Canton et al. 1985)
EC50 values to crustaceans, mg/l	> 77.1 5.4 16	48hr, mbt, Daphnia magna (Pearson et al. 1979) immobilisation, 48hr, Daphnia manga (Canton et al. 1983) 24hr, Daphnia magna (Bringmann et al. 1982)
LOEC values to crustaceans, mg/l	10	21d, semi-static (Deneer et al. 1989)
LC50 values to fishes, mg/l	38 0.1–49.7 37.1 33 29 88	96hr, Pimephales promelas (Pearson et al. 1979) 96hr, Pimephales promelas (Bailey & Spanggord 1983) 96hr, Pimephales promelas (Liu et al. 1983) 14d, Poecilia reticulata (Deneer et al. 1987) 48hr, Leuciscus idus (Juhnke et al. 1978) 48hr, Oryzias latipes (MITI 1992)

Other information about water organisms	LOEC 24 mg/l, rpd, schr, Uronema parduczi (Bringmann & Kühn 1980b). EC50 (24hr), 100 mg/l, rpd, Tetrahymena pyriformis (Yoshioka et al. 1985). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 28 mg/l protozoa (Entosiphon sulcatum): 46 mg/l (Bringmann & Kühn 1980a)

1510 • p-Nitrotoluene

99-99-0

Synonyms	4-Methylnitrobenzene p-Methylnitrobenzene 4-Nitrotoluene	
Sumformula of the chemical	C7H7NO2	
Melting point, °C	51.3	(MITI 1992)
Boiling point, °C	238.3	(MITI 1992)
Log octanol/water coefficient, log Pow	2.42	(Sangster 1989)
Total degradation in water	Biodegradation: 0.8% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).	
Bioconcentration factor, fishes	3.7–7.2 4.5–8.0	6w, Cyprinus carpio, conc 0.1 mg/l 6w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
Effects on amphibia	NOEC, 10 mg/l, 100d, Xenopus laevis, mortality. NOEC, 3.2 mg/l, 100d, Xenopus laevis, development. NOEC, 32 mg/l, 100d, Xenopus laevis, growth. (Slooff & Canton 1983)	
Effects on arthropods	NOEC, 3.2 mg/l, 25d, Culex pipiens, mortality. NOEC, 3.2 mg/l, 25d, Culex pipiens, development. (Slooff & Canton 1983)	
Effects on plants	NOEC, 10 mg/l, 7d, Lemna minor, specific growth rate. (Slooff & Canton 1983)	
Effects on microorganisms	NOEC, 10 mg/l, 0,3d, Pseudomonas fluorescens, specific growth rate. NOEC, 3.2 mg/l, 4d, Microcystis aeruginosa, specific growth rate. (Slooff & Canton 1983) Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 26 mg/l (Bringmann & Kühn 1980a)	
LOEC values to algae, mg/l	3.3	rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
NOEC values to algae, mg/l	10	4d, grw (biomass), Scenedesmus pannonicus (Slooff & Canton 1983)
EC50 values to crustaceans, mg/l	12.1	48hr, Daphnia magna (Pearson et al. 1979)
NOEC values to crustaceans, mg/l	3.2 1	21d, srv, Daphnia magna (Slooff & Canton 1983) 21d, rpd, Daphnia magna (Slooff & Canton 1983)

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LC50 values to fishes, mg/l	49.9 74	96hr, Pimephales promelas (Pearson et al. 1979) 48hr, Oryzias latipes (MITI 1992)
NOEC values to fishes, mg/l	10 10 10 1 1 32	28d, srv, Poecilia reticulata 28d, srv + bhv, Poecilia reticulata 28d, grw, Poecilia reticulata 40d, srv, Oryzias latipes 40d, srv + bhv, Oryzias latipes 40d, grw, Oryzias latipes (Slooff & Canton 1983)
Other information about water organisms	LOEC 8.6 mg/l, rpd, schr, Entosiphon sulcatum (Bringmann & Kühn 1980a). EC50 (24hr), 82 mg/l, rpd, Tetrahymena pyriformis (Yoshioka et al. 1985). NOEC, 10 mg/l, 21d, Hydra oligactis, specific growth rate. NOEC, 10 mg/l, 40d, Lymnaea stagnalis, mortality. NOEC, 0.32 mg/l, 40d, Lymnaea stagnalis, reproduction. NOEC, 10 mg/l, 40d, Lymnaea stagnalis, hatching. (Slooff & Canton 1983). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 15 mg/l protozoa (Entosiphon sulcatum): 8.6 mg/l (Bringmann & Kühn 1980a).	

1511 • Nonadecanenitrile 28623-46-3

Synonyms	n-Nonadecanenitrile	
Water solubility, mg/l	< 10	(MITI 1992)
Melting point, °C	41–43	(MITI 1992)
Total degradation in water	Biodegradation: 89–96% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	

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1512 • Nonadecyl amine 14130-05-3

Sumformula of the chemical	C19H41N	
Water solubility, mg/l	< 10	(MITI 1992)
Melting point, °C	51.5–55	(MITI 1992)
Boiling point, °C	175	4 mmHg (MITI 1992)
Total degradation in water	Biodegradation: 47–76% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

1513 • Nonaeicosane 630-03-5

Synonyms	Nonacosane
Sumformula of the chemical	C29H60
EINECS-number	2111262
Water solubility, mg/l	< 1 mg/l (MITI 1992)
Melting point, °C	63.6–64.1 (MITI 1992)
Boiling point, °C	346–348 40 mmHg (MITI 1992)
Total degradation in water	Biodegradation: 42–67% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

1514 • Nonane 111-84-2

Use	Solvent.	
Boiling point, °C	150.8	
Log octanol/water coefficient, log Pow	5.65	(Sangster 1989)
Henry's law constant, Pa x m³/mol	601100	calc. (Yaws et al. 1991)
Volatilization	Relative volatility (nBuAc=1) = 0.40	

1515 • 1-Nonanol 143-08-8

Synonyms	Nonyl alcohol	
Sumformula of the chemical	C9H20O	
Log octanol/water coefficient, log Pow	4.02	(Sangster 1989)
Henry's law constant, Pa x m³/mol	1.675	calc. (Yaws et al. 1991)
EC50 values to microorganism, mg/l	519	Biodegradation inhibition (Vaishnav 1986)
LC50 values to crustaceans, mg/l	25	96hr, 21 °C, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	5.7	96hr, Pimephales promelas (Veith et al. 1983)
	18	96hr, 10 °C, Alburnus alburnus (Linden et al. 1979)
	5.5	96hr, Pimephales promelas (Broderius & Kahl 1985)
	16	24hr, Carassius auratus (Bridie et al. 1979)

1516 • 1-Nonene 124-11-8

Synonyms	Propylenetrimer
Sumformula of the chemical	C9H18

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EINECS-number	2046817	
Water solubility, mg/l	< 100	(MITI 1992)
Melting point, °C	< -50	(MITI 1992)
Boiling point, °C	45–145	(MITI 1992)
Total degradation in water	Biodegradation: 0–1% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	906–2230 995–1940	8w, Cyprinus carpio, conc 0.02 mg/l 8w, Cyprinus carpio, conc 0.002 mg/l (MITI 1992)
LC50 values to fishes, mg/l	1.5	48hr, Oryzias latipes (MITI 1992)

1517 • β-n-Nonenylsuccinic anhydride 28928-97-4

Synonyms	1-Nonen-2-ylsuccinic acid anhydride	
Chemical oxygen demand, g 02/g	2.23	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.25	5 days (Bridie et al. 1979)
LC50 values to fishes, mg/l	310 10	pH 7, 24hr, Carassius auratus pH 5, 24hr, Carassius auratus (Bridie et al. 1979)

1518 • Nonylphenol 104-40-5 * 4-nonylphenol
25154-52-3 * mixture

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Synonyms	p-Nonylphenol Nonyl phenol 4-Nonylphenol	
Sumformula of the chemical	C15H24O	
Use	Non-ionic surfactant (nonbiodegradable), lube oil additives, stabilizers, petroleum demulsifiers, fungicides, antioxidants for plastics and rubber. Raw material in manufacturing of nonylphenolethoxylate tensides (NFE) which is used in detergents and cleansers mostly in industrial use and industrial laundries.	
Molecular weight	220.39	
Density, kg/m³	950 949	20 °C, CAS 104-40-5 20 °C, CAS 25154-52-3
Water solubility, mg/l	5	20-25 °C, CAS 25154-52-3 insignificant, CAS 104-40-5
Boiling point, °C	315 295–320 292.8–297.2 (MITI 1992)	CAS 104-40-5 CAS 25154-52-3
Log octanol/water coefficient, log Pow	3.01 3.28 4.2	CAS 104-40-5 pH7, CAS 104-40-5 CAS 104-40-5 (Anon. 1989)

Mobility	Theoretical distribution: 25% in water, > 60% in sediment, > 10% in soil (Anon. 1989).
Aerobic degradation in soil	Degradation of aromatic ring 95% in 48 days in soil (Schöberl 1985). Degradion in soil 3 months after spreading of sludge: approximately 92% (Diercxsens & Tarradellas 1987). A mixture of root sludge, compost and sandy soil: degradation in 40 days: 89%, 100 ppm; 62%, 1000 ppm at 25 °C (Trocm` et al. 1988).
Aerobic degradation in water	No aerobic degradation in 135 hours (1 mg/l) in household waste water whereas 45% degradation occurred in the same time period in industrial waste water (Gaffney 1976).
Total degradation in water	Biodegradaation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Other information about degradation	Adaptation of microorganism flora is needed (Gaffney 1976). After adaption (43 days) in Modified Sturm test: 56% aerobic degradation in 20 days, 78% in 40 days (Schöberl 1985). No anaerobic degradation (Gieger et al. 1984).
Bioconcentration factor, fishes	100 carp (Kawasaki 1980) 75–280 4d, salmon (McLeese et al. 1981) 2.5–3.3 8w, Cyprinus carpio, conc 0.1 mg/l 0.9–2.2 8w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Bioconcentration factor, mollusca	1.4–13 4d, Mytilus (McLeese et al. 1980) 3000 mussel (Ekelund et al. 1988)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	1620 orl-rat (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	2140 skn-rbt (Sweet 1987)
Other information about mammals	Skin and eye irritation data: skin, rabbit, 10 mg, 24hr, open, severe; skin, rabbit, 500 mg, open, moderate; eye, rabbit 0.050 mg, open, severe (Sweet 1987).
EC50 values to algae, mg/l	1.5 24hr, Chlorella (Weinberger & Rea 1982)
LC50 values to crustaceans, mg/l	0.3–0.4 96hr, Crangon (McLeese et al. 1981) 0.2 96hr, Homarus (McLeese et al. 1980)
EC50 values to crustaceans, mg/l	0.18 24hr, Daphnia magna (Bringmann & Kühn 1982) 0.14–0.19 24hr, Daphnia pulex (Ernst et al. 1980)

MNO

LC50 values to fishes, mg/l	0.13–0.9	96hr, juv., Salmo salar (McLeese et al. 1980)
	0.135	96hr, Pimephales promelas (Holcombe et al. 1984)
	0.48–0.92	96hr, Salmo gairdneri (Ernst et al. 1980)
	0.145	96hr, Salvelinus, McLeese et al. 1980
	0.95	48hr, Oryzias latipes (MITI 1992)
Other information about water organisms	Tetrahymena pyriformis, EC50, 24hr, 0.46 mg/l, rpd (Yoshioka et al. 1985). Mytilus, LC50: 96hr, 3.0 mg/l; 850hr, 0.14 mg/l (Granmo et al. 1989). Fish, sublethal effects, 0.1 mg/l (Holcombe et al. 1984).	

1519 • Nonylphenol ethoxylates 9016-45-9

Synonyms	NFE AFE Alkylphenol ethoxylate Polyoxyethylene p-nonylphenyl ether
Sumformula of the chemical	Rn-C6H4OH(EO)m * see other phys.&chem. prop.
Products containing the chemical	Lubrol APN 5 Nonidet NP 50
Use	AFE is used as a component in detergents mostly in industry (NFE up to 10 EO groups), in washing up liquid (NFE with about 20 EO), in emulgators (NFE) with about 30 EO), in dispersers (NFE with up to about 80 EO).
Density, kg/m³	1010–1100, 20 °C
Water solubility, mg/l	> 1000 (MITI 1992)
Melting point, °C	42–43 (MITI 1992)
Log octanol/water coefficient, log Pow	> 4, NFE(4-16 EO) Other physicochemical properties: Sumformula: Rn-C6H4OH(EO)m R = branched alkylgroup EO = ethyleneoxide: CH2CH2O; m = 2–approx. 80
Total degradation in water	Biodegradation: 0% by BOD period: 21d substance: 30 mg/l sludge: 30 mg/l (MITI 1992).
Degradation and transformation products	NFE with high amount of EO degrades to NF4-NFO (4-nonylfenol)(4-0 EO grourp) (Granmo et al. 1986). Nonylphenoxyacetic acid is another possible degradation product (Granmo et al. 1986).
Other information about degradation	NFE (10–15), 10–30% in 1–2 days in refinery (model plant); NFE (3–30 EO), 90% in 12 days in refinery (model plant); NFE (3–30 EO), 30% in 60 days in river water; NFE (2 EO), 80% in 28 days (Swedmark 1986). The technical mixture does not undergo full biological degradation only the splitting of ethoxylates (see 4-nonylphenol) (Swedmark 1986). Swiss refinery: 50% of NFE converts into nonylphenol and accumulates in anaerobic sludge (Brunner et al. 1988).
Bioconcentration factor, fishes	< 0.2 6w, Cyprinus carpio, conc 2 mg/l < 1.4 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)

MNO

Other information about bioaccumulation	Octanol/water-partion coefficient and thus propably the bioaccumulation potential increases with decreasing amount of EO groups in the molecule (Hedenmark 1987).
LD50 values to mammals in oral exposure, mg/kg	2600 orl-rat, NFE (3 EO) (Hedenmark 1987) 800–6600 1orl-mus, gpg, rat, NFE (10 EO) (Swedmark 1986)
Effects on wastewater treatment	Disturbances in biological step at refineries up from 1 mg/l NFE (9EO) (Malmqvist & Duus 1989).
LC50 values to crustaceans, mg/l	33–100 48hr, Lubrol APN 5, Crangon crangon (Kemp et al. 1973)
LC50 values to fishes, mg/l	6 96hr, Gadus morrhua, NFE (9-10 EO) 5 96hr, Gasterosteus aculeatus, NFE (9-10) 5–9 96hr, marine fish, NFE (4 EO) 6 96hr, marine fish, NFE (10 EO) > 400 96hr, marine fish, NFE (40 EO) (Swedmark 1986) 1 96hr, Salmo trutta, NFE (9-10 EO) 8.6 96hr, Rasbora, NFE (9-10 EO) 7–11.2 96hr, Idus idus, NFE (9-10 EO) 4.9 48hr, Carassius auratus, NFE (9-10 EO) (Hedenmark 1987) 12.5 sfd, 48hr, Lubrol APN 5 16 hrd, 48hr, Rasbora heteromorpha (Kemp et al. 1973) 7 96hr, Nonidet NP 50, Carassius auratus (Anon. 1975) > 1000 48hr, Oryzias latipes (MITI 1992)
Other information about water organisms	LC50, marine mussels, 96hr, NFE (10 EO), < 5 → 100 mg/l (Swedmark 1986). NFE (10 EO): Fish: impaired development of eggs, swimming activity (96hr), growth, reproduction (200 days): 0.1–0.5; crustacea: mobility, growth (200 days), 0.1–< 1 mg/l; mussels, effects on fertility, 0.05 mg/l, 24hr (Swedmark 1986).

1520 • Norbormide 991-42-4

Other information about mammals	ALD = 28 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987).
LD50 values to birds in oral exposure, mg/kg	> 100 orl-Agelaius phoeniceus > 100 orl-Sturnus vulgaris (Schafer et al. 1983)

1521 • Norflurazon 27314-13-2

Use	Herbicide.
Effects on plants	Tubers of Cyperus rotundus L. were planted to soil sprayed with 2.0 kg norflurazon/ha → a decrease in weight of nutsedge (C. rotundus) sprouts above ground (6 weeks after treatment) (Rincon & Warren 1979).

MNO

1522 • 2,3,3,3,2',3',3',3'-Octachloro-di-propylether 127-90-2

Sumformula of the chemical	C6H6Cl80
EINECS-number	2048704
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	900–6900 8w, Cyprinus carpio, conc 0.010 mg/l 500–3300 8w, Cyprinus carpio, conc 0.001 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be accumulated on a medium level (Anon. 1987).
LC50 values to fishes, mg/l	4.2 48hr, Oryzias latipes (MITI 1992)

1523 • Octachloronaphthalene 2234-13-1

LC50 values to crustaceans, mg/l	> 530 48hr, Daphnia magna (LeBlanc 1980)

1524 • Octachlorostyrene 29082-74-4

Synonyms	Octachlorovinylbenzene
Sumformula of the chemical	C8Cl8
Molecular weight	379.71
Water solubility, mg/l	0.06 calc. 20 °C
Log octanol/water coefficient, log Pow	6.29 (Anon. 1989) 7.68
Other information about degradation	In UV-light > 290 nm, extremely slow photolysis (Hustert et al. 1984).
Bioconcentration factor, fishes	10000–1000000 fish (Ernst et al. 1984)
Bioconcentration factor, other organisms	3.5–6.7 oligochaeta, towards sediment, 110 days (Oliver 1984)
Other information about mammals	Mammals, NOEL, 0.5 mg/kg in birth, same kind of effects as with hexachlorobenzene (Tarkpea et al. 1985).
Mutagenicity	Negative in Ames test with and without metabolic activation (Kaminsky & Hites 1984).
LC50 values to crustaceans, mg/l	0.068 96hr, Nitocra spinipes, Tarkpea et al.1985
Other information	Is produced as biproduct in electrolysis with graphite electrodes, e.g. when manufacturing magnesium and in aluminium smelteries. Biproduct in manufacturing of tetrachloroethene and carbontetrachloride.

MNO

1525 • Octadecanethiol 2885-00-9

Sumformula of the chemical	C18H38S
Water solubility, mg/l	< 15000 (MITI 1992)
Melting point, °C	27.7 (MITI 1992)
Boiling point, °C	176-178 2 mmHg (MITI 1992)
Log octanol/water coefficient, log Pow	> 5.60 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.3 6w, Cyprinus carpio, conc 0.5 mg/l < 2.8 6w, Cyprinus carpio, conc 0.05mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 300 48hr, Oryzias latipes (MITI 1992)

1526 • Octadecenylsuccinic acid 28299-29-8

Water solubility, mg/l	0.03 (MITI 1992)
Melting point, °C	71.6–73.4 (MITI 1992)
Log octanol/water coefficient, log Pow	> 4.4 (MITI 1992)
Bioconcentration factor, fishes	0.1–0.4 6w, Cyprinus carpio, conc 0.5 mg/l < 1.3–2.0 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 250 48hr, Oryzias latipes (MITI 1992)

MNO

1527 • Octadecenylsuccinic anhydride 28777-98-2

Sumformula of the chemical	C22H38O3
Melting point, °C	65.3–69.0
Total degradation in water	Biodegradation: 4–10% by BOD (hydrolyzed to Octadecenylsuccinic acid) period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

1528 • Octadecyl methacrylate 32360-05-7

Water solubility, mg/l	< 1 mg/l (MITI 1992)
Melting point, °C	20–21 (MITI 1992)

Total degradation in water	Biodegradation: 87% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

1529 • N-n-Octadecyl-N,N-dimethyl amine 124-28-7

Synonyms	N,N-Dimethyl-1-octadecanamine
Sumformula of the chemical	C20H43N
EINECS-number	2046948
Water solubility, mg/l	0.44 (MITI 1992)
Melting point, °C	21 (MITI 1992)
Boiling point, °C	> 300 (MITI 1992)
Total degradation in water	Biodegradation: 46–72% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).

1530 • Octadecylisocyanate 112-96-9

Sumformula of the chemical	C19H37NO
EINECS-number	2040197
Melting point, °C	20 (MITI 1992)
Boiling point, °C	300 atmospheric pressure (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD (altered to N,N'-Dioctadecylurea) period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

MNO

1531 • Octamethylpyrophosphoramide 152-16-9

Other information about mammals	ALD = 8.0–12.0 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987).
LD50 values to birds in oral exposure, mg/kg	11.0–12.0 orl-Sturnus vulgaris (Schafer et al. 1983)

1532 • Octane 111-65-9

Use	Solvent.
Boiling point, °C	125.6

Log octanol/water coefficient, log Pow	5.15 (Sangster 1989)
Henry's law constant, Pa x m³/mol	499500 calc. (Yaws et al. 1991)
Volatilization	Relative volatility (nBuAc=1) = 1.23

1533 • 1-Octanol

111-87-5

Synonyms	n-Octanol Octanol	
Sumformula of the chemical	C8H18O	
Use	Perfumery, cosmetics, organic synthesis, solvent manufacture of high-boiling esters, antifoaming agent, flavouring agent.	
State and appearance	Colourless liquid.	
Odour	Penetrating aromatic odour.	
Specific gravity (water=1)	0.826	20 °C
Boiling point, °C	194–195 °C	
Flashing point, °C	81.1	
Log octanol/water coefficient, log Pow	3.1 3.07	(Anon. 1986) (Sangster 1989)
Other physicochemical properties	Miscible with alcohol, chloroform, mineral oil; immiscible with water and glycerol. Combustible.	
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): > 50 mg/l (Bringmann & Kühn 1980a).	
EC50 values to microorganism, mg/l	625 4.7 5.9	Biodegradation inhibition (Vaishnav 1986) 15 min Microtox (Hermens et al. 1985) Microtox (Tarkpea et al. 1986)
LOEC values to algae, mg/l	1.9 6.3	rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976) rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
LC50 values to crustaceans, mg/l	58	96hr, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	15–17 12–15 17.68	96hr, Alburnus alburnus (Linden et al. 1979) 96hr, Pimephales promelas (Broderius & Kahl 1985) 4d, Salmo gairdneri (McKim et al. 1987)
Other information about water organisms	Salmo gairdneri, lethal threshold concentration (LT50): 15.84 mg/l, 0.23 d (McKim et al. 1987). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 6.3 mg/l protozoa (Entosiphon sulcatum): 44 mg/l (Bringmann & Kühn 1980a).	

1534 • 2-Octanol

123-96-6

EC50 values to microorganism, mg/l	651	Biodegradation inhibition (Vaishnav 1986)

MNO

1535 • 2-Octanone

111-13-7

Log octanol/water coefficient, log Pow	2.37	(Sangster 1989)
EC50 values to microorganisms, mg/l	1667	Biodegradation inhibition (Vaishnav 1986)
LC50 values to fishes, mg/l	35–63	96hr, Pimephales promelas (Broderius & Kahl 1985)

1536 • 3-Octanone

106-68-3

Synonyms	Ethyl amyl ketone
Molecular weight	128.24
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 25 mg/l (Bringmann & Kühn 1980a).
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 53 mg/l protozoa (Entosiphon sulcatum): 256 mg/l (Bringmann & Kühn 1980a).

1537 • Octyl acrylate

103-11-7

Synonyms	2-Ethylhexyl acrylate	
Odour	Quality: musty, sharp Hedonic tone: unpleasant Threshold odour concentration absolute: 0.073 ppm 50% recognition: 0.18 ppm 100% recognition: 0.18 ppm Odour Index 100% recognition: 7 333 (Hellman & Small 1974).	
Water solubility, mg/l	0.01	(MITI 1992)
Melting point, °C	< -90	(MITI 1992)
Boiling point, °C	213.5	(MITI 1992)
Total degradation in water	Biodegradation: 51% by BOD (on the upward trend) period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	

1538 • n-Octyl cyanide

2243-27-8

Synonyms	Nonanenitrile 1-Cyanooctane n-Nonanenitrile Nonanonitrile Octyl cyanide 1-Octyl cyanide Pelargonitrile

MNO

Sumformula of the chemical	C9H17N
Water solubility, mg/l	70 (MITI 1992)
Total degradation in water	Biodegradation: 60–74% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	2059 orl-mus (Sweet 1987)
LC50 values to fishes, mg/l	6.9 96hr, Pimephales promelas (Broderius & Kahl 1985)

1539 • p-Octyldiphenylamine 4175-37-5

LC50 values to fishes, mg/l	> 40 48hr, Carassius auratus (McKee & Wolf 1963)

1540 • 4-Octyloxy-2-hydroxy-benzophenone 1843-05-6

Synonyms	2-Hydroxy-4-n-octoxybenzophenone
Melting point, °C	48 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	1.5–35 8w, Cyprinus carpio, conc 0.5 mg/l 18–140 8w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	> 100 48hr, Oryzias latipes (MITI 1992)

1541 • 4-Octylphenol 1806-26-4

Synonyms	p-Octylphenol
Melting point, °C	80.5–81.5 (MITI 1992)
Boiling point, °C	276 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

Bioconcentration factor, fishes	113–469 8w, Cyprinus carpio, conc 0.1 mg/l 12–135 8w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	1.05 48hr, Oryzias latipes (MITI 1992)

1542 • Oleic acid

112-80-1

State and appearance	Colourless needles.	
Molecular weight	282.52	
Vapour pressure, mmHg	1	177 °C
Melting point, °C	14	
Boiling point, °C	360	
LD50 values to mammals in oral exposure, mg/kg	74	orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	230	ivn-mus (Lewis & Sweet 1984)
LC50 values to fishes, mg/l	8	Na-, act, Carassius auratus (Bock 1967)
	205	96hr, Pimephales promelas (Vincent et al. 1976)

1543 • Omacide-24 *

15922-78-8

Chemicals in the product	Sodium salt of pyrithion	
Use	Fungicide.	
LC50 values to fishes, mg/l	0.054	96hr, Rasbora heteromorpha (Tooby et al. 1975)

MNO

1544 • Optunal

23422-53-9

Other information about mammals	ALD = 94.0 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987).

1545 • 7-Oxabicyclo(2,2,1)heptane-2,3-dicarboxylic acid

145-73-3

Synonyms	Aquathol 1,2-Dicarboxy-3,6-endoxocyclohexane 3,6-Endoxohexahydrophthalic acid Endothal
Sumformula of the chemical	C8H1005
Use	Herbicide; defoliant; desiccant; growth regulator.
Molecular weight	186.18
Water solubility, mg/l	100000 at 20 °C
Melting point, °C	144

Effects on arthropods	Insects: lowest observed avoidance concentration: > 10 mg/l (dipotassium salt), mayfly nymphs (Ephemerella walkeri) (Folmar 1978).
LC50 values to fishes, mg/l	160 96hr, dipotassium salt Lepomis macrochirus 320 96hr, dipotassium salt Pimephales promelas (Surber & Pickering 1962)

Other information about water organisms

Algae:	ppb		
Chlorococcum sp.	technical acid	100000	50% decrease in 02 evolution
Chlorococcum sp.	technical acid	50000	50% decrease in growth
Dunaliella tertiolecta	technical acid	425000	50% decrease in 02 evolution
Dunaliella tertiolecta	technical acid	50000	50% decrease in growth
Isochrysis galbana	technical acid	60000	50% decrease in 02 evolution
Isochrysis galbana	technical acid	25000	50% decrease in growth
Phaeodactylum tricornutum	technical acid	75000	50% decrease in 02 evolution
Phaeodactylum tricornutum	technical acid	15000	50% decrease in growth
Chlorococcum sp.	amine salt	> 1000000	50% decrease in 02 evolution
Chlorococcum sp.	amine salt	300000	50% decrease in growth
Dunaliella tertiolecta	amine salt	> 1000000	50% decrease in 02 evolution
Dunaliella tertiolecta	amine salt	45000	50% decrease in growth
Isochrysis galbana	amine salt	> 1000000	50% decrease in 02 evolution
Isochrysis galbana	amine salt	22500	50% decrease in growth
Phaeodactylum tricornutum	amine salt	> 1000000	50% decrease in 02 evolution
Phaeodactylum tricornutum	amine salt	25000	50% decrease in growth

(growth measured as ABS (525 mu) after 10 days) (Walsh 1972).

Crustacean: Gammarus lacustris: no effect at 100 ml /96hr (dipotassium salt) (Sanders 1969).

Fish: Rainbow trout (Salmo gairdneri): lowest observed avoidance concentration: > 10 mg/l (dipotassium salt) (Folmar 1978).

1546 • Oxadiazon 19666-30-9

Synonyms	2-tert-Butyl-4-(2,4-dichloro-5-isopropoxyphenyl)-1,3,4-oxadiazolin-5-one	
Use	Herbicide.	
Water solubility, mg/l	7	(MITI 1992)
Melting point, °C	90	(MITI 1992)

Total degradation in water	Biodegradation: 16% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	24.1–26.7 8w, Cyprinus carpi, conc 0.04 mg/l 2.48–2.87 8w, Cyprinus carpio, conc 0.004 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
Effects on plants	Weed groundcover of Ischaemum afrum was controlled by pre-planting herbicides in green-ridged groundnut: 1.12 kg oxadiazon/ha was applied with a sprayer → a decrease in weed groundcover (Jennings & Drennan 1979).
LC50 values to fishes, mg/l	8.4 48hr, Oryzias latipes (MITI 1992)

1547 • Oxalic acid 144-62-7

Sumformula of the chemical	C2H2O4
Molecular weight	90.04
Water solubility, mg/l	400000 22 °C (Suntio et al. 1988)
Melting point, °C	101–102 (Suntio et al. 1988)
pKa	1.27 (Suntio et al. 1988)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 1550 mg/l (Bringmann & Kühn 1980a).
LOEC values to algae, mg/l	80 rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 790 mg/l protozoa (Entosiphon sulcatum): 222 mg/l (Bringmann & Kühn 1980a)
Other information	Toxicity is based on the acidity.

1548 • Oxycarboxin 5259-88-1

Use	Fungicide.
LC50 values to fishes, mg/l	28.1 96hr, Lepomis macrochirus 19.9 96hr, Salmo gairdneri (Pesticide Manual 1983)

1549 • Oxydemeton-methyl 301-12-2

Synonyms	Metasystox-R Demeton-O-methylsulfokside S-(2-(Ethylsulfinyl)-ethyl)-O,O-dimethylphosphorothioate
Use	Active ingredient in insecticides.
Molecular weight	230.3
Melting point, °C	< -10

Boiling point, °C	106	
LD50 values to mammals in oral exposure, mg/kg	30	orl-rat, orl-mus (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	100	skn-rat (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	15 42	orl-pgn orl-bwd (Lewis & Sweet 1984)
LC50 values to crustaceans, mg/l	0.19	96hr, Gammarus lacustris (Sanders 1969)
LC50 values to fishes, mg/l	4 10 10	96hr, Salmo gairdneri (Walker 1964) 24hr, Salmo gairdneri 24hr, Lepomis macrochirus (Pesticide Manual 1983)
Other information about water organisms	LC50 (96hr) 0.035 mg/l, Pteronarcys californica (Sanders & Cope 1968).	

1550 • Ozone

10028-15-6

Molecular weight	48	
LC50 values to mammals in inhalation exposure, ppm	4.8	0.01 mg/l, 4hr, ihl-rat (Lewis & Sweet 1984) TCLo values to mammals in inhalation exposure, ppm0.2: 3hr, ihl-hmn (Lewis & Sweet 1984)
Effects on plants	A commercial field corn (Zea mays) hybrid was exposed to chronical doses of 03 in open-top field chambers from 25 days after planting until maturity. The threshold 03 concentrations causing foliar imjury were between 0.02 and 0.07 ppm (Heagle et al. 1979)	
LC50 values to fishes, mg/l	0.0093 0.21 0.19–0.31 0.06	96hr, Salmo gairdneri (Wedemeyer et al. 1979) embryo, 24hr, Perca flavescens embryo, Salmo gairdneri (Coler & Asbury 1980) 24hr, Lepomis macrochirus (Paller & Heidinger 1979)

1551 • Palmitic acid

57-10-3

Sumformula of the chemical	C16H3202	
pKa	4.5	est. (Sangster 1989)
Log octanol/water coefficient, log Pow	7.17	(Sangster 1989)
Other information about water organisms	LC 11 mg/l, act, Carassius auratus (Bock 1967).	

1552 • Palustric resin acid

1945-53-5

LC50 values to fishes, mg/l	0.55 0.32	96hr, Salmo gairdneri (Anon. 1981) 96hr, Salmo gairdneri (Leach & Thakore 1978)

1553 • Panacide * 97-23-4

Synonyms	2,2'-Dihydroxy-5,5'-dichlorodiphenylmethane
Active ingredients	Dichlorophen * 40%
Use	Slimicide.
Water solubility, mg/l	34 (MITI 1992)
Melting point, °C	177–178 (MITI 1992)
Log octanol/water coefficient, log Pow	4.96 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	26–84 8w, Cyprinus carpio, conc 0.05 mg/l 98–281 8w, Cyprinus carpio, conc 0.005 mg/l (MITI 1992)
LC50 values to crustaceans, mg/l	5 72hr, Asellus (Landner et al. 1973)
LC50 values to fishes, mg/l	0.5 24hr, Rasbora heteromorpha 3.8 24hr, Poecilia reticulata (Landner et al. 1973) 1.35 48hr, Oryzias latipes (MITI 1992)
Other information about water organisms	LC50 (72hr), 1.5 mg/l, Anodonta cygnea (Landner et al. 1973).

1554 • Paraclox R 80 * 34911-46-1

Active ingredients	4-Hydroxy-2-oxophenylacethydroximic acid chloride * 10%
Use	Pesticide; slimicide.
LC50 values to crustaceans, mg/l	1.07 96hr, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	14.5 96hr, Alburnus alburnus (Linden et al. 1979)

1555 • Paraffin 8002-74-2

Use	Active ingredient in insecticides.
TDLo values to mammals in non-oral exposure, mg/kg	480 implant-mus, tumorigenic 120 implant-rat, tumorigenic (Sweet 1987)

1556 • Paraformaldehyde 30525-89-4

Synonyms	Formaldehyde polymer Polyformaldehyde
Sumformula of the chemical	(CH2O)X

State and appearance	White crystalline powder.
Odour	Odour of formaldehyde.
Melting point, °C	120–170 (HSDB 1995)
Other physicochemical properties	Slowly soluble in cold water, more readily soluble in hot water. Insoluble in most organic solvents. The higher polymers are insoluble in water. The rate at which paraformaldehyde dissolves (hydrolyses) in water is at a minimum at pH 3–5; it increases rapidly at lower or higher pHs (HSDB 1995).
LD50 values to mammals in oral exposure, mg/kg	800 orl, rat (OHMTADS 1995)
LC50 values to fishes, mg/l	60 96hr, Salmo gairdneri (Sprague & Logan 1979) 60 96hr, Oncorhynchus mykiss (AQUIRE 1995)

1557 • Paraquat

1910-42-5

Synonyms	1,1'-Dimethyl-4,4'-bipyridinium dichloride Dextrone N,N'-Dimethyl-4,4'-bipyridinium dichloride 4,4'-Dimethyldipyridyl dichloride 1,1'-Dimethyl-4,4'-dipyridylium chloride Dimethyl viologenchloride Paraquat chloride
Sumformula of the chemical	C12H14N2.2Cl
Use	Herbicide.
Molecular weight	257.18
Water solubility, mg/l	> 1000 (MITI 1992)
Aerobic degradation in soil	No significant degradation in sterile or nonsterile soil incubated aerobically for 90 days (25 °C) (Verschueren 1983).
Anaerobic degradation in soil	No significant degradation in sterile or nonsterile soil incubated anaerobically for 90 days (25 °C) (Verschueren 1983).
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.2–0.3 6w, Cyprinus carpio, conc 2 mg/l < 1.9 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	57 orl-rat 22 orl-gpg 25 orl-dog (Lewis & Sweet 1984) 35 orl-cat 30 orl-domestic animal 50 orl-mky 120 orl-mus 30 orl-pig (Sweet 1987)

LD50 values to mammals in non-oral exposure, mg/kg	80	skn-rat (Lewis & Sweet 1984)
	3	ipr-gpg
	30	ipr-mus
	26	ipr-rat
	18	ipr-rbr
	1	ivn-domestic animal
	180	ivn-mus
	21	ivn-rat
	24	scu-rat
	325	skn-rbt
		(Sweet 1987)
LDLo values to mammals in oral exposure, mg/kg	214	orl-hmn
	43	orl-man
	3000	orl-wmn
	111	orl-wmn
		(Sweet 1987)
LDLo values to mammals in non-oral exposure, mg/kg	34.5	ivn-dog (Sweet 1987)
TDLo values to mammals in oral exposure, mg/kg	32	orl-man (Lewis & Sweet 1984)
TDLo values to mammals in non-oral exposure, mg/kg	30.15	ipr-mus, 8-16d preg. effects on fertility
	6.5	ipr-mus, 6d preg. specific developmental abnormalities (Sweet 1987)
Other information about mammals	Skin and eye irritation data: eye, rabbit, 25 mg, mild (Sweet 1987).	
Mutagenicity	Mutation data: cytogenic analysis: hamster, lung, 3mmol/l; DNA inhibition: rat, orl, 126 mg/kg; DNA repair: S. typhimurium, 0.1 mg/plate; unscheduled DNA synthesis: human, fibroblast, 20 mg/l; human, cell types, 20 mg/l; gene conversion and mitotic recombination: S. cerevisiae, 100 ppm; microbial mutation withour S9: A. nidulans, 0.4 mg/plate; microorganisms, 1000 ppm; S. typhimurium 2500 ng/plate: microsomal assay: S. typhimurium; 0.02 mg/plate; sex chromosome loss and nondisjunction: A. nidulans. 20000 mg/l; sister chromatid exchange: hamster, fibroblast, 1 mmol/l; hamster, lung, 0.1 mmol/l; test systems (other): chicken, liver, 50 mg/l; rat, orl, 126 mg/l (Sweet 1987).	

PQR

LD50 values to birds in oral exposure, mg/kg	199 362	orl-dck orl-ckn (Lewis & Sweet 1984)
LD50 values to birds in dermal exposure, mg/kg	600	skn-dck (Lewis & Sweet 1984)
Effects on plants	34 days old nutgrass (Cyperus rotundus) plants were sprayed with paraquat dichloride at the equivalent of 0.28 kg/ha (ion) → e.g. rapid necrosis of green shoots, shoot dry weights declined, some decay and loss of dry weight of rhizomes and roots occurred (Hammerton 1974). Beans (Phaseolus vulgaris) wee sprayed to 'run off' at the fully expanded primary leaf stage. Paraquat at 0.00025 M increased leaf–cell membrane permeability after exposure for 12hr or less (Prendeville & Warren 1977). Growth of oat roots was inhibited by 50% during 72hr of paraquat treatment at 21 ppm (Coffey & Warren 1969).	
LOEC values to algae, mg/l	5	10d, rpd, Isochyris galbana (Walsh 1972)
LC50 values to crustaceans, mg/l	3.7 > 40	48hr, Daphnia pulex (Sanders & Cope 1966) act, Daphnia pulex (Hashimoto & Nishiuchi 1981)
LC50 values to fishes, mg/l	32	96hr, Salmo gairdneri (Pesticide Manual 1983)
	2.5–13	96hr, Salmo trutta m. lacustris (Pesticide Manual 1983)
	62	96hr, Salmo gairdneri (Edwards 1977)
	7 12	96hr, Rasbora trilineata 96hr, Poecilia reticulata (Kam-Wing & Furtado 1977)
	76	96hr, Oncorhynchus kisutch (Lorz et al. 1979)
	604	96hr, Gambusia affinis (Johnson 1978)
	840	24hr, Rasbora heteromorpha (Alabaster 1969)
	> 40 > 10	48hr, Cyprinus carpio 48hr, Carassius auratus (Hashimoto & Nishiuchi 1981)
	593	48hr, Oryzias latipes (MITI 1992)
Effects on the physiology of water organisms	Cyprinus carpio, 5.0 mg/l, 1 d, change in enzyme activity (Vig et al. 1987).	

1558 • PCB

1336-36-3

Synonyms	Polychlorinated biphenyls
Products containing the chemical	Clophen Aroclor 1262 Aroclor 1323 Aroclor 1232 Aroclor 1016 * see PCB Aroclor 1016 Aroclor 1221 * see PCB Aroclor 1221 Aroclor 1242 * see PCB Aroclor 1242 Aroclor 1248 * see PCB Aroclor 1248 Aroclor 1254 * see PCB Aroclor 1254 Aroclor 1260 * see PCB Aroclor 1260
Chemicals in the product	* Aroclor 1262 1232; *; chlorine * 62% 32%
Use	In heat transfer, hydraulic fluids, lubricants and insecticides.

PQR

State and appearance	A series of technical mixtures consisting of many isomers and compounds that vary from mobile oily liquids to white crystalline solids and hard noncrystalline resins. Technical products vary in composition, in the degree of chlorination and possibly according to batch.
Water solubility, mg/l	0.052 24 °C, Aroclor 1262
Boiling point, °C	340–375
Log octanol/water coefficient, log Pow	5–7 (Anon. 1989) 4–8,3 (Anon. 1986b)
Bioconcentration factor, mammals	13000000 sea water/dolphin (Virtanen & Nuuja 1987)
Bioconcentration factor, crustaceans	6400 sea water/zoopl. (Virtanen & Nuuja 1987)
Degradation and transformation products	Chlorinated dibenzofurans
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Other information about degradation	Photolytic dechlorination has been indicated (Crosby & Moilanen 1973). In water solution photochemical degradation can produce chlorinated dibenzofurans (Crosby & Moilanen 1973). Low chlorinated components degrade aerobically. For example Aroclor 1221 in 30 days (Wong & Kaiser 1975). Anaerobic degradation occurs only by selected bacteria cultures, except for 2,4,2',4'-tetrachlorobiphenyl (Chen et al. 1988).
Metabolism in mammals	Effective uptake in alimentary canal. Is metabolized for instance to toxic methylsulfones (Anon. 1989).
Other information about bioaccumulation	Confirmed to be accumulated on a high level (Anon. 1987). No unambiguous biomagnification in food chain of water organisms – clear biomagnification in terrestrial animals (Landner & Skoglund 1977).
LD50 values to mammals in oral exposure, mg/kg	1900 orl-mus (Sax 1989)
LD50 values to mammals in non-oral exposure, mg/kg	4000–11000 ukn-rat (Virtanen & Nuuja 1987) 500 ukn-mink, Arochlor 1254 (Virtanen & Nuuja 1987)
TDLo values to mammals in oral exposure, mg/kg	325 orl-mam 16800 orl-rat (Sax 1989)
Effects on the reproduction of mammals	Effects on the reproduction of seals and sea lions together with high PCB concentrations (IJC 1977).
Other information about mammals	Mink, orl, 9.9 mg/d, 22 d, lethal effects (Kihlström et al. 1976).
Health effects	Moderately toxic by ingestion. Some are poisons by other routes. Suspected human carcinogens. Experimental carcinogens and tumorigens. Experimental reproductive effects. Two distinct actions on the body, a skin effect and a toxic action on the liver. The higher the chlorine content of the diphenyl compound, the more toxic is it liable to be (Sax 1989).
Carcinogenicity	Induction of liver tumors in mice with high doses (Tomic et al. 1973).
Effects on the reproduction of mammals	5–11 mg/kg prevented reproduction of mink (Virtanen & Nuuja 1987); 20 mg/kg was lethal.
Health effects	Lowest lethal dose (man): 500 mg/kg (Virtanen & Nuuja 1987).
Effects on microorganisms	EC50, Aroclor 1016, 2.050 mg/l, 5 min (Anon. 1986b) EC50, Aroclor 1221, 0.009 mg/l, 5 min (Anon. 1986b) EC50, Aroclor 1242, 0.700 mg/l, 5 min (Anon. 1986b)

LC50 values to crustaceans, mg/l	0.010–0.073 mg/l, LC50/EC50, Gammarus spec. (Anon. 1986b) 0.03–0.1 Clophen A30, 48hr, Crangon crangon 1.0–3.3, Clophen A40, 48hr, Crangon crangon 3.3 –10, Clophen A50, 48hr, Crangon crangon (Kemp et al. 1973)
EC50 values to crustaceans, mg/l	0.010–0.073 mg/l, LC50/EC50, Gammarus spec. (Anon. 1988)
LC50 values to fishes, mg/l	0.002 96hr, Salmo gairdneri 0.0023 96hr, Micropterus salmoides 0.0077–0.300 mg/l, 96hr, Pimephales promelas 0.0087–0.139 mg/l, 30d, Ictalurus punctatus 0.084–0.400 mg/l, 30d, Lepomis macrochirus (Anon. 1986b) 2.5 96hr, Salmo clarci (Mayer et al. 1977) 0.32 96hr, Rasbora heteromorpha (Tooby et al.75)
Effects on the reproduction of water organisms	Effects on reproduction, Clophen A 60, Brachydanio, 0.001 mg/l (Kihlström et al. 1977).
Other information about water organisms	Aroclor 1262: Harlequin fish: 96hr LC10: not toxic below 100 mg/l (Tooby et al. 1975).

1559 • PCB Aroclor 1016 * 12674-11-2

Chemicals in the product	Chlorine * 16%
Water solubility, mg/l	0.22–0.25
Other physicochemical properties	Composition of the water soluble fraction (WSF): monochloro isomers * 12.2% of WSF dichloro isomers * 30.9% of WSF trichloro isomers * 36.3% of WSF tetrachloro isomers * 20.6% or WSF (Lee et al. 1979). Partition coefficient to natural sediments:

	physicochemical characteristics of sediment					
sediment	*TOC, %*	*pH*	*% sand*	*% salt*	*% clay*	*part.c*
USDA Pond	0.8	6.4	-	-	-	1370
Doe Run Pond	1.4	6.1	56.0	44.0	< 1.0	1290
Hick.Hill.P.	2.4	6.3	55.0	45.0	< 1.0	1300
Oconee River	0.4	6.5	93.0	6.0	2.0	620

(Steen et al. 1978).

Bioconcentration factor, fishes	13000 Ermyzon oblongus 10600 Perca flavescens 14700 Lepomis gibbosus 22300 Ictalurus nebulosus 17000 Ictalurus nebulosus (Skea et al. 1979)
LC50 values to fishes, mg/l	0.012 4d, larvae, Ictalurus punctatus 0.0011 4d, larvae, Salmo gairdneri (Birge et al. 1978)
Effects on the physiology of water organisms	Salmo gairdneri; 2 mg/l, 4 days; enzyme effect (change in enzyme activity (Castren & Oikari 1987).

PQR

1560 • PCB Aroclor 1221 * 11104-28-2

Chemicals in the product	Chlorine * 21%
Water solubility, mg/l	0.59 at 24 °C
Other physicochemical properties	Composition of the water soluble fraction (WSF): monochloro isomers * 92.2% WSF dichloro isomers * 6.6% WSF trichloro isomers * 0.9% WSF tetrachloro isomers * 0.3% WSF (Lee et al. 1979).
LC50 values to fishes, mg/l	1.2 96hr, Salmo clarci (Mayer et al.1977) 1.05 96hr, Rasbora heteromorpha (Tooby et al. 1975)

1561 • PCB Aroclor 1232 11141-16-5

Chemicals in the product	Chlorine * 32%
LC50 values to fishes, mg/l	2.5 96hr, Salmo clarci (Mayer et al. 1977) 0.32 96hr, Rasbora heteromorpha (Tooby et al. 1975)

1562 • PCB Aroclor 1242 * 53469-21-9

Chemicals in the product	monochlorobiphenyls * 3%; dichlorobiphenyls * 13%; trichlorobiphenyls * 28%; tetrachlorobiphenyls * 30%; pentachlorobiphenyls * 22%; hexachlorobiphenyls * 4%
Use	Dielectric liquids; thermostatic fluids; swelling agents for transmission seals; additives or base for lubricants, oils and greases; plasticizers for cellulosics, vinyls and chlorinated rubbers.
Specific gravity (water=1)	1.41 at 65/15.5 °C
Vapour pressure, mmHg	50 at 225 °C
Water solubility, mg/l	0.1 at 24 °C
Other physicochemical properties	Composition of the water soluble fraction (WSF): monochloro isomers * 19.4% of WSF dichloro isomers * 31.8% of WSF trichloro isomers * 31.3% of WSF tetrachloro isomers * 16.5% of WSF pentachloro isomers * 0.9 / of WSF (Lee et al. 1979). Partition coefficient to natural sediments:

	physico-chemical characteristics of sediment					
sediment	*TOC (%)*	*pH*	*% sand*	*% salt*	*% clay*	*part.c*
USDA Pond	0.8	6.4	-	-	-	1210
Doe Run Pond	1.4	6.1	56.0	44.0	< 1.0	1090
Hick.Hill.P.	2.4	6.3	55.0	45.0	< 1.0	1250
Oconee River	0.4	6.5	93.0	6.0	2.0	540

(Steen et al. 1978).

Half-life in water, days	0.5 12.1hr, calculated half-life based on evaporative loss for a water depht of 1 m at 25 °C, MacKay & Leinonen 1975.
Bioconcentration factor, fishes	32000–274000, Pimephales promelas after 8 months exposure (Anon. 1977).

PCB

Effects on arthropods	Naiad of damselfly (Ischnura verticalis): 4 days LC50: 0.40 mg/l Naiad of dragonfly (Macromia sp.): 7 days LC50: 0.80 mg/l (Mayer et al. 1977).	
EC50 values to algae, mg/l	0.007	24hr, marine phytoplankton (Moore & Harris 1972)
LC50 values to crustaceans, mg/l	0.03 0.01	7 days, Orconectes nais 4 d, Gammarus fasciatus (Mayer et al. 1974)
NOEC values to crustaceans, mg/l	0.02	rpd, schr, Daphnia magna (Nebeker & Puglisi 1974)
LC50 values to fishes, mg/l	0.067 0.012 0.084 0.087 5.4	5d, Salmo gairdneri 25d, Salmo gaidneri 30d, Lepomis macrochirus 30d, Ictalurus punctatus 96hr, Salmo clarci (Mayer et al. 1977)
	0.37	96hr, Rasbora heteromorpha (Tooby et al. 1975)
	0.0043 0.001	4d, Ictalurus punctatus, larvae 4d, Salmo gairdneri, larvae (Birge et al. 1978)
LOEC values to fishes, mg/l	0.015	srv, chr, Pimephales promelas (Nebeker et al. 1974)
NOEC values to fishes, mg/l	0.005	srv, chr, Pimephales promelas (Nebeker et al. 1974)

1563 • PCB Aroclor 1248 * 12672-29-6

Chemicals in the product	Chlorine * 48%; dichlorobiphenyls * 2%; trichlorobiphenyls * 18 %; tetrachlorobiphenyls * 40%; pentachlorobiphenyls * 36%; hexachlorobiphenyls * 4%	
Use	In the electrical industry in capacitors and transformers; in the formulation of lubricating and cutting oils.	
Water solubility, mg/l	0.1	20 °C (Anon. 1989)
	The solubility of PCB decreases with increasing chlorination (0.04-0.2 ppm) (Verschueren 1983).	
Half-life in water, days	0.397	= 9.53hr, calculated, based on evaporative loss, depht 1 m, 25 °C (MacKay & Leinonen 1975)
Bioconcentration factor, fishes	60000–120000	8 months, Pimephales promelas (Anon. 1977)
	56370 120000	77d, Ictalurus punctatus Pimephales promelas (Verschueren 1983)
LD50 values to mammals in oral exposure, mg/kg	11000	orl-rat (Lewis & Sweet 1984)
LDLo values to mammals in non-oral exposure, mg/kg	1269	skn-rbt (Lewis & Sweet 1984)
LC50 values to crustaceans, mg/l	0.052	96hr, Gammarus (Mayer et al. 1977)
NOEC values to crustaceans, mg/l	0.001	rpd, schr, Daphnia magna (Nebeker & Puglisi 1974)

PQR

LC50 values to fishes, mg/l	> 1.5 0.075 5.7 0.078 0.136 0.0034 0.054	act, Salmo gairdneri 30d, Salmo clarci 96hr, Salmo clarci 30d, Lepomis macrochirus 5d, Lepomis macrochirus 25d, Salmo gairdneri 5d, Salmo gairdneri (Mayer et al.1977)
LOEC values to fishes, mg/l	0.003 0.005 0.005	srv, grw, chr, Pimephales promelas (Defoe et al.1978) srv, grw, chr, Pimephales promelas srv, grw, chr, flag fish (Nebeker et al. 1974)
NOEC values to fishes, mg/l	0.001 0.002 0.002	srv, grw, chr, Pimephales promelas (Defoe et al. 1978) srv, grw, chr, Pimephales promelas srv, grw, chr, flag fish (Nebeker et al. 1974)

1564 • PCB Aroclor 1254 * 11097-69-1

Chemicals in the product	chlorine * 54%; tetrachlorobiphenyls * 11%; pentachlorobiphenyls * 49%; hexachlorobiphenyls * 34%; heptachlorobiphenyls * 6%
Use	In the electrical industry in capacitors and transformers; in the formulation of lubricating and cutting oils.
Water solubility, mg/l	0.057 24 °C 0.05 20 °C (Anon. 1989) The solubility of PCB decreases with increasing chlorination (0.04–0.2 ppm) (Verschueren 1983). Composition of the water soluble fraction (WSF): trichlorobiphenyls * 2.6% of WSF tetrachlorobiphenyls * 40.2% of WSF penta and hexabiphenyls * 57.2% of WSF (Lee et al. 1979).
Half-life in water, days	0.43 10.3hr, calculated half-life based on evaporative loss for a water depth of 1 m at 25 °C (MacKay & Leinonen 1975)
Other information about degradation	Biodegradation (0.05 mg/l): 0% after 135hr (normal sewage); 43% after 135hr (adapted sewage) (Verschueren 1983). Impact on biodegradation processes: effect on degradation of glucose by mixed culture derived from activated sludge: *conc. (mg/l)* / *increase in lag period/ hours* / *espiration rate* 1 / 0 / 100 10 / 0 / 110 100 / 0 / 135 1000 / > 200 / 0 (Verschueren 1983). Degradation decreases strongly when chlorination stage increases; Aroclor 1254 is persistent (Wong & Kaiser 1975)

PQR

Bioconcentration factor, fishes	6500 after 7 days, Ictalurus punctatus 61190 after 77 days (Mayer et al. 1977) 109000–238000 244d, Pimephales promelas (Verschueren 1983) 46000–307000 8 months, Pimephales promelas (Anon. 1977) 40000–47000 Salvelinus fontinalis (Mauck et al. 1978) 34000–46000 30 days, Salmo gairdneri (Verchueren 1983)
Bioconcentration factor, crustaceans	160–6300 (Verschueren 1983) 3800 4 days, daphnid 750 21 days, crayfish 2600 21 days, grass shrimp (Mayer et al. 1977)
Bioconcentration factor, other organisms	740 21 days, stonefly 1500 21 days, dobsonfly 3500 7 days, mosquito 2700 14 days, phantom midge (Mayer et al. 1977)
Other information about mammals	Dietary exposure to 5–800 ppm can inhibit the growth of at least one experimental tumor, the Walker 256 carcinosarcoma. Continuous feeding of Aroclor 1254 in a diet produced varying degrees of dermatitis after 10 weeks. These skin lesions were found in 15 of 60 animals fed th PCB at 100 ppm, 4 of 60 at 30 ppm, and 1 of 60 at 10 ppm for 10 to 20 weeks (Verschueren 1983).
Carcinogenicity	NCI carcinogenesis bioassay completed: results indefinite; rat (Lewis & Sweet 1984). It is concluded that under the conditions of this bioassay, Aroclor 1254 was not carcinogenic in Fischer 344 rats; however, a high incidence of hepatocellular proliferative lesions in both male and female rats was related to administration of the chemical. In addition, the carcinomas of the gastrointestinal tract may be associated with administration of Aroclor 1254 in both males and females (Verschueren 1983).
Effects on arthropods	Naiad of damselfly (Ischnura verticalis): 4 days LC50: 0.20 mg/l; naiad of dragonfly (Macromia sp.): 7 days LC50: 1.0 mg/l (Mayer et al. 1977).
EC50 values to algae, mg/l	0.015 24hr, marine phytoplanktons (Moore & Harris 1972)
LC50 values to crustaceans, mg/l	0.00094 15d, Penaeus duorarum (Mayer et al. 1977) 2.4 4 days, Gammarus fasciatus 0.1 7 days, Orconectes nais 0.003 7 days, Palaemonetes kadiakensis (Stahl 1979)
NOEC values to crustaceans, mg/l	0.001 rpd, schr, Daphnia magna (Nebeker & Puglisi 1974)
LC50 values to fishes, mg/l	0.139 30d, Ictalurus punctatus 0.177 30d, Lepomis macrochirus 0.027 25d, Salmo gairdneri (Tooby et al. 1975) 0.0063 128d, Salvelinus fontinalis (Mauck et al. 1978) 3.2 5 days, Coregonus, 22-day-old fry (Verschueren 1983) 0.142 5d, Salmo gairdneri (Mayer & Ellersieck 1986)
LOEC values to fishes, mg/l	0.0003 srv, schr, Cyprinodon variegetus (Schimmel et al.1974) 0.005 srv, grw, schr, Pimephales promelas (Nebeker et al. 1974)

PQR

NOEC values to fishes, mg/l	0.0001 srv, schr, Cyprinodon variegetus (Schimmel et al. 1974) 0.002 srv, grw, schr, Pimephales promelas (Nebeker et al. 1974) < 0.00043 Salvelinus (Manck et al. 1978)
Effects on the physiology of water organisms	Ctenopharyngodon idella; Cyprinus carpio; Tinca tinca: 50 mg/kg, 2 days; cytogenetic effect (changes in the RNA and DNA of the cell) (Al-Sabti 1986). Salmo gairdneri, 0.003 mg/g, 180 days, hematological effect (change in various blood parameters such as red blood cell count, hematocrit, and serum osmolarity) (Chen et al. 1986). Ictalurus punctatus, 4 d, 50 mg/kg, enzyme effect (Ankley & Blazer 1988). Salmo gairdneri; 50 d, 500 µg/g, food consumption rate (Spitsbergen et al. 1988); 360 d, 30–300 mg/l, growth effect (Cleland et al. 1988).
Effects on the reproduction of water organisms	Effects on reproduction, Cyprinodon, 0.0001 mg/l (Schimmel et al. 1974).
Other information about water organisms	Tetrahymena pyriformis: 10 ppb, 13.3% decrease in population size, 96hr static lab bioassay (Verschueren 1983). Crustaceans: Penaeus duorarum 0.94 ppb 51% mortality 15 day chronic exposure in flowing seawater Penaeus duorarum 3.5 ppb 50% mortality 35 day chronic exposure in flowing seawater Leiostomus xanthurus 5 ppb 50% mortality 18 day chronic exposure in flowing seawater Lagodon rhomboides 5 ppb 50% mortality 12 day chronic exposure in flowing seawater (Stahl 1979).

1565 • PCB Aroclor 1260 * 11096-82-5

Chemicals in the product	Chlorine * 60%; pentachlorobiphenyls * 12%; hexachlorobiphenyls * 38%; heptachlorobiphenyls * 41%; octachlorobiphenyls * 8%; nonachlorobiphenyls * 1%
Water solubility, mg/l	0.08 at 24 °C 0.025 20 °C (Anon. 1989)
Half-life in water, days	0.425 10.2hr, calculated half-life based on evaporative loss for a water depth of 1 m at 25 °C (MacKay & Leinonen 1975)
Bioconcentration factor, fishes	270000 250 d, Pimephales promelas (DeFoe et al. 1978)
NOEC values to crustaceans, mg/l	0.01 rpd, schr, Daphnia magna (Nebeker & Puglisi 1974)
LC50 values to fishes, mg/l	0.433 30d, Ictalurus punctatus 0.0033 30d, Pimephales promelas 0.4 30d, Lepomis macrochirus 0.051 30d, Salmo gairdneri (Defoe et al. 1978) 0.24 10d, Salmo gairdneri (Stalling & Mayer 1972)
LOEC values to fishes, mg/l	0.004 srv, grw, chr, Pimephales promelas (Defoe et al. 1978)
NOEC values to fishes, mg/l	0.001 srv, grw, chr, Pimephales promelas (Defoe et al. 1978)

PQR

Other information about water organisms	Rainbow trout: acute oral toxicity: > 1.5 g/kg (Mayer et al. 1977).	

1566 • Pebulate 1114-71-2

Use	Herbicide.	
Log soil sorption coefficient, log Kom	2.8	(Sabljic 1987)
LD50 values to birds in oral exposure, mg/kg	> 100 > 100	orl-Agelaius phoeniceus orl-Sturnus vulgaris (Schafer et al. 1983)
LC50 values to crustaceans, mg/l	10	96hr, Gammarus fasciatus (Sanders 1970)
LC50 values to fishes, mg/l	7.4	96hr, Salmo gairdneri Lepomis macrochirus (Anon. 1969)

1567 • 1,2,3,4,5-Pentabromo-6-chlorocyclohexane 87-84-3

Sumformula of the chemical	$C_6H_6Br_5Cl$	
EINECS-number	2017765	
Water solubility, mg/l	< 10	(MITI 1992)
Log octanol/water coefficient, log Pow	4.72	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	76–534 125–388	8w, Cyprinus carpio, conc 0.025 mg/l 8w, Cyprinus carpio, conc 0.0025 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 50	48hr, Oryzias latipes (MITI 1992)

1568 • Pentabromophenol 608-71-9

Other information about water organisms	Tetrahymena pyriformis, LC50, grw, 2d, 1.06 mg/l (Schultz 1987).

1569 • Pentabromotoluene 87-83-2

Water solubility, mg/l	< 2	(MITI 1992)
Melting point, °C	285–291	(MITI 1992)
Log octanol/water coefficient, log Pow	5.43	(MITI 1992)

PQR

Total degradation in water	Biodegradation: 7% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	4.5–39 6w, Cyprinus carpio, conc 0.01 mg/l < 4.5–34 6w, Cyprinus carpio, conc 0.001 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	> 5 48hr, Oryzias latipes (MITI 1992)

1570 • Pentachlorobenzene 608-93-5

Sumformula of the chemical	C6HCl5
Use	Intermediate.
Molecular weight	250.32
Water solubility, mg/l	0.24 22 °C 0.831 25 °C (Miller et al. 1984) 1.33 25 °C (Banerjee et al. 1980) 0.12 (MITI 1992)
Melting point, °C	86 (Suntio et al. 1988) 85 (MITI 1992)
Boiling point, °C	275–277 (MITI 1992)
Log octanol/water coefficient, log Pow	4.88–5.69 (Sabljic 1987) 5.19 observed (Chin et al. 1986) 5.19 (Anon. 1988) 5.79 (Yalkowsky 1979) 4.88 (Konemann et al. 1979) 5.69 (Konemann et al. 1979) 4.94 (Banerjee et al. 1980) 5.17 (Wateral et al. 1982) 5.03 (Miller et al. 1984) 5.2 (Chiou 1985) 5.7 (Banerjee et al. 1984) 5.19 (Mackay 1982) 5.2 (MITI 1992)
Henry's law constant, Pa x m³/mol	66 (Anon. 1988) 85 calc. (Suntio et al. 1988)
Mobility	Equilibrium distribution: *mass %* air 48.10 water 2.10 solid 49.81 (Anon. 1988).
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

PQR

Bioconcentration factor, fishes	260000	(Verschueren 1983)
	1430-6840	8w, Cyprinus carpio, conc 0.01 mg/l
	1130-5070	8w, Cyprinus carpio, conc 0.001 mg/l (MITI 1992)
Bioconcentration factor, other organisms	16000	approx. 16000 (Verschueren 1983)
LD50 values to mammals in oral exposure, mg/kg	1080	orl-rat (Lewis & Sweet 1984)
LC50 values to crustaceans, mg/l	5.3	48hr, Daphnia magna (LeBlanc 1980)
	0.11	16d, Daphnia magna (Hermens et al. 1984)
	0.24	21d, Daphnia magna (van Leeuwen et al. 1987)
EC50 values to crustaceans, mg/l	0.025	rpd, 16 d, Daphnia magna (Hermens et al. 1984)
	0.12	Daphnia magna (van Leeuwen et al. 1987)
NOEC values to crustaceans, mg/l	0.1	16d, srv, Daphnia magna (Hermens et al. 1984)
	0.01	16d, rpd, Daphnia magna (Hermens et al. 1984)
LC50 values to fishes, mg/l	0.25	96hr, Lepomis macrochirus (Buccafusco et al. 1981)
	0.18	14 d, Poecilia reticulata (Könemann 1979)
	0.8	96hr, Cyprinodon variegatus (Heitmuller et al. 1981)
	0.27	144hr, a mixture with dimethylforamide, Salmo gairdneri (USEPA 1984)
	2.76	48hr, Oryzias latipes (MITI 1992)
EC50 values to fishes, mg/l	0.1	144hr, a mixture with dimethylforamide, Salmo gairdneri (USEPA 1984)
NOEC values to fishes, mg/l	0.0549	32d, Pimephales promelas (USEPA 1984)

1571 • Pentachlorobiphenyl 25429-29-2

LC50 values to crustaceans, mg/l	0.21	96hr, Gammarus fasciatus (Mayer et al. 1977)

1572 • Pentachloroethane 76-01-7

Synonyms	Ethane pentachloride	
Use	Solvent for oil and grease in metal cleaning.	
Vapour pressure, mmHg	3.4	20 °C
Melting point, °C	-29	
Boiling point, °C	161–162	
Henry's law constant, Pa x m³/mol	183.9	calc. (Yaws et al. 1991)
Bioconcentration factor, fishes	62	32d, Pimephales promelas (USEPA 1984)
LDLo values to mammals in oral exposure, mg/kg	500	orl-dog (Lewis & Sweet 1984)
LCLo values to mammals in inhalation exposure, mg/kg	35	2hr, ihl-mus (Lewis & Sweet 1984)
LCLo values to mammals in inhalation exposure, ppm	4238	2hr, ihl-rat (Lewis & Sweet 1984)

PQR

Carcinogenicity	NTP carcinogenesis bioassay completed: results positive, mus; results negative, rat (Lewis & Sweet 1984).	
LC50 values to crustaceans, mg/l	63	48hr, Daphnia magna (LeBlanc 1980)
	7.32	48hr, unfed, Daphnia magna
	8.02	48hr, fed, Daphnia magna (USEPA 1984)
EC50 values to crustaceans, mg/l	4.69	48hr, unfed, Daphnia magna
	6.88	48hr, fed, Daphnia magna (USEPA 1984)
LC50 values to fishes, mg/l	7.2	96hr, Lepomis macrochirus (Buccafusco et al. 1981)
	15	7d, Poecilia reticulata (Könemann 1979)
	7.3	96hr, Pimephales promelas (Veith et al. 1983)
	116	96hr, Cyprinodon variegatus (Heitmuller et al. 1981)
	7.34	96hr, flow-through, Pimephales promelas (USEPA 1984)
NOEC values to fishes, mg/l	0.9–1.4	32d, Pimephales promelas (USEPA 1984)

1573 • Pentachlorophenol 87-86-5

Sumformula of the chemical	C6HCl5O	
Products containing the chemical	DOW EC-7 Dowicide G * sodium pentachlorophenate 79% * sodium salts of chlorophenols 11%	
Known impurities	Chlorinated predioxins * anddibenzofurans * in technical products (Jensen & Renberg 1972).	
Use	Insecticide, algicide, herbicide, fungicide, wood impregnant; blacide; disinfectant.	
State and appearance	White monoclinic, crystalline solid, technical grade dark grey to brown.	
Molecular weight	266.32	
Density, kg/m³	1978	22 °C
Vapour pressure, mmHg	0.00011	20 °C
Water solubility, mg/l	14	20 °C, pH 5 (Anon. 1986b)
	14	25 °C, pH 5.3 (Blackman et al. 1967)
	2000	20 °C, pH 7 (Anon. 1989)
	77.2	(MITI 1992)
Melting point, °C	174	(Suntio et al. 1988)
	190–191	(MITI 1992)
Boiling point, °C	309	(Anon. 1986b)
	309–310	(MITI 1992)
Degradation point, °C	310	
pKa	5.25–4.92	(Doedens 1967)
	4.7	25 °C (Anon. 1988)

PQR

Log octanol/water coefficient, log Pow	3.32–5.86	(Sabljic 1987)
	5.01	observed (Chin et al. 1986)
	3.65	pH 7 (Anon. 1986b)
	5.01	(Anon. 1988)
	5.06	(Xie 1984)
	5.12	(Hansch & Leo 1979)
	3.81	(Lu & Metcalf 1975)
	2.5	(Geyer et al. 1987)
	3.69	(Geyer et al. 1982)
	5.01	(Mackay 1982)
	5	pH2 (Anon. 1989)
	4.2	pH7 (Anon. 1989)
Log soil sorption coefficient, log Kom	3.73	observed (Sabljic 1987)
	3.46	calculated (Sabljic 1987)
Henry's law constant, Pa x m³/mol	0.29	(Anon. 1988)
	0.2615	calc. (Suntio et al. 1988)
Mobility	2.43% (air), 32.95% (water), 64.62% (sediment). Equilibrium distribution:	
		mass %
	air	0.58
	water	5.95
	solid	93.47
		(Anon. 1988).
	Theoretical distribution: approx. 35% in water; approx. 50% in sediment and > 10% in soil (Nordic 1988).	
Photochemical degradation in air	Photochemical degradation in UV-light (290–330 nm) (Jensen & Renberg 1972).	
Other reactions in atmosphere	Chlorinated dioxins are formed in fires (Anon. 1989).	
Photochemical degradation in water	In water, half-life 10 days, chloranil and predioxines are formed (Jensen & Renberg 1972).	
Half-life in soil, days	48	(Li et al. 1990)
Aerobic degradation in soil	AEROBIC DEGRADATION IN SOIL Maximum adsorption wavelength: 322 nm NON-STERILE SOIL Minimum time for > 70% decrease: 88.0–160.0 d % decomposition at the termination of the experiment: 160d, 80% STERILE SOIL % decomposition at the termination of the experiment: 160d, 20% (Baker et al. 1980).	
Anaerobic degradation in soil	ANAEROBIC DEGRADATION IN SOIL Maximum adsorption wavelength: 322 nm NON-STERILE SOIL % decomposition at the termination of the experiment: 160d, 7% STERILE SOIL % decomposition at the termination of the experiment: 160d, 5% (Baker et al. 1980).	
Aerobic degradation in water	Aerobic degradation in water: 16%, 7 days, long lag phase Aerobic degradation in water: after adaption, 99%, 28 days (Tabak et al. 1981).	
Anaerobic degradation in water	Anaerobic degradation in sludge: reductive dechlorination (Rippen 1988).	

PQR

Total degradation in soil	Biodegradation: decomposition rate in soil suspensions: > 72 days for complete disappearance (Verschueren 1983). In soil, degradation in 2 months (Rippen 1988).
Total degradation in water	OECD Screening test: 5%, 28 days (Rippen 1988). Negative in MITI test (Anon. 1989). Biodegradation: 1% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992)
Degradation and transformation products	Pentachloroanisole * strongly bioaccumulative, toxic and with odour; polychlorinated dibenzodioxins * when heated (pyrolysis).
Other information about degradation	Degradation by Pseudomonas (200 mg/l, 30 °C): parent: 7% ring disruption in 120hr mutant: 26% ring disruption in 120hr (Verschueren 1983). Degradation of pentachlorophenol:

ENVIRONMENT	*INIT.CONC. mg/l*	*REDOX-COND.*	*TEMP. °C*	*DEGRADATION %/day*	*REF.*
water	5	aerobic	25	19/7	a
water (adapted)	5	aerobic	25	100/21	a
water (adapted)	50	aerobic	4	11-52/100	b
water (adapted)	50	aerobic	20	50-56/12	b
water (adapted)	–	aerobic	–	100/1	c
sludge	0.6	methanogen	36	95/7	d
sludge	1.2	methanogen	36	72/7	d
sludge	2.4	methanogen	36	< 10/7	d
sludge	2.4	methanogen	36	75/30	d
sludge	6.0	methanogen	36	< 10/7	d
sludge	6.0	methanogen	36	0/30	d
sludge	12.5	anaerobic	37	100/14	e
sludge	12.5	anaerobic	37	100/29	e
sludge (2-CP-ad.)	10	anaerobic	37	100/3	f
sludge (3-CP-ad.)	10	anaerobic	37	46/7	f
sludge (4-CP-ad.)	10	anaerobic	30	71/7	f
soil suspension	10–100	aerobic	30	100/72	g
soil	100	aerobic	28	80/28	h
soil	100	anaerobic	28	95/28	h
soil	–	anaerobic	–	66/24	i
soil	–	anaerobic	–	15/24	i
soil	1	aerobic	23	80/160	k
sterile soil	1	aerobic	23	20/160	k
soil	1	anaerobic	23	7/80	k
sterile soil	1	anaerobic	23	5/80	k
soil (adapted)	10	aerobic	30	60/11	l
soil (adapted)	100	aerobic	30	70/11	l
soil (adapted)	500	aerobic	30	0/11	l
soil (adapted)	100	aerobic	12	0/11	l
soil (adapted)	100	aerobic	24	42/14	l
soil (adapted)	100	aerobic	30	50/15	l
soil (adapted)	100	aerobic	35	36/14	l

PQR

	a) Tabak et al. 1981 b) Trevors 1982 c) Steiert & Crawford 1985 d) Suflita & Miller 1985 e) Mikesell & Boyd 1985 f) Mikesell & Boyd 1986 g) Alexander & Aleem 1961 h) Ide et al. 1972 i) Murthy et al. 1979 k) Baker & Mayfield 1980 l) Crawford & Mohn 1985 (Anon. 1987b).
Bioconcentration factor, fishes	475 (Verschueren 1983) 1000 5d, Carassius auratus (Anon. 1986b) 13 8d, Lepomis macrochirus (Anon. 1986b) 770 32d, Pimephales promelas (Rippen 1988) 300 three-spines stickleback 100 flounder (Jensen & Renberg 1974) 39–198 8w, Cyprinus carpio, conc 0.03 mg/l 45–224 8w, Cyprinus carpio, conc 0.003 mg/l (MITI 1992)
Bioconcentration factor, algae	1250 Chlorella, 24hr (Freitag et al. 1982)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	50 orl-rat (Lewis & Sweet 1984) 27–28 orl-rat (Verschueren 1983) 74 orl-mus (Ahlborg & Thunberg 1980)
LD50 values to mammals in non-oral exposure, mg/kg	105 skn-rat (Lewis & Sweet 1984) 11.7 ihl-rat (Hoben et al. 1976)
LDLo values to mammals in oral exposure, mg/kg	29 orl-hmn (Lewis & Sweet 1984)
LDLo values to mammals in non-oral exposure, mg/kg	40 skn-rbt (Lewis & Sweet 1984)
Other information about mammals	Rat, NOEL, 2 years, female 3 mg/kg/d, male 10 mg/kg/d (Schwetz et al. 1978). Strongly embryotoxic (Crosby 1981).
Health effects	Strongly irritating to skin and eyes (Jensen & Renberg 1972).
Carcinogenicity	No mutagenic or carcinogenic effects has been shown with the pure PCP (IARC 1979).
LD50 values to birds in oral exposure, mg/kg	380 orl-dck (Lewis & Sweet 1984)
Effects on amphibia	NOEC, 0.032 mg/l, 100d, Xenopus laevis, mortality. NOEC, 0.032 mg/l, 100d, Xenopus laevis, development. NOEC, 0.032 mg/l, 100d, Xenopus laevis, growth. (Slooff & Canton 1983)
Effects on arthropods	NOEC, 3.2 mg/l, 25d, Culex pipiens, mortality. NOEC, 3.2 mg/l, 25d, Culex pipiens, development. (Slooff & Canton 1983)
Effects on plants	NOEC, 1 mg/l, 7d, Lemna minor, specific growth rate. (Slooff & Canton 1983)
Effects on microorganisms	EC50, Photobacterium phosphoreum, 0.370 mg/l, 30 min, EC50, Photobacterium phosphoreum, 0.760 mg/l, 15 min, EC50, Photobacterium phosphoreum, 0.500 mg/l, 5 min (Anon. 1986b) NOEC, 1 mg/l, 0.3d, Pseudomonas fluorescens, specific growth rate. NOEC, 1 mg/l, 4d, Microcystis aeruginosa, specific growth rate. (Slooff & Canton 1983)

PQR

EC50 values to microorganism, mg/l	8 9 6.5 11	0.5hr Resazurin reduction, methanol 0.5hr Resazurin reduction, ethanol 0.5hr Resazurin reduction, acetone 0.5hr Resazurin reduction, DMSO (Thompson et al. 1986)
	19–55	3hr Act. sludge respiration (King and Painter 1986)
	1	15 min Microtox (Nacci et al. 1986)
	1	Microtox (Tarkpea et al. 1986)
	1.5	Microtox (Vasseur et al. 1986)
	1	Microtox (20 °C) (Vasseur et al. 1986)
	24	OECD 209 (King and Painter 1985)
	36	16hr Growth (King and Painter 1985)
	2.5	OECD 209 (Klecka et al. 1985)
EC50 values to algae, mg/l	0.09	96hr, grw, Scenedesmus subspicatus (Geyer et al. 1985)
	0.8 0.09	48hr, Scenedesmus subspicatus, chlorose 96hr, Lemna minor (Anon. 1986b)
NOEC values to algae, mg/l	0.1	rpd, 96hr, Scenedesmus pannonicus (Slooff & Canton 1983)
	0.1	4d, grw (biomass), Scenedesmus pannonicus (Slooff & Canton 1983)
LC50 values to crustaceans, mg/l	0.48 2 1.5	48hr, Daphnia magna 48hr, Daphnia pulex 48hr, Daphnia cucullata (Canton & Adema 1978)
	0.68 1.5	48hr, Daphnia magna 24hr, Daphnia magna (LeBlanc 1980)
	0.48	48hr, Daphnia magna (Pesticide Manual 1983)
	1.2–1.7 0.6–1.0	24hr, Daphnia magna 48hr, Daphnia magna (Adema 1978)
	3.6	act, Daphnia pulex (Hashimoto & Nishiuchi 1981)
	0.48	act, Daphnia magna (Kenaga 1979)
	0.8	21d, Daphnia magna van (Leeuwen et al. 1987)
	1.15–1.37	4d, Gammarus pseudolimnaeus (Graney et al. 1987)
	0.475 0.6 2 0.44	Daphnia magna 48hr, Daphnia magna Daphnia pulex 14d Daphnia magna (Anon. 1986b)
	2.9 0.7	48hr, Asellus aquaticus (Slooff 1983) 48hr, Gammarus pulex (Slooff 1983)
	0.27	96hr, brackish water, Nitocra (Linden et al. 1979)
	0.092 0.48	96hr, pH6.5, Gammarus 96hr, pH8, Gammarus (Spehar et al.1985)
EC50 values to crustaceans, mg/l	0.23	Daphnia magna (van Leeuwen et al. 1987)
	0.48	48hr, Daphnia magna (Canton & Adema 1978)

PQR

NOEC values to crustaceans, mg/l	0.1	21d, srv, Daphnia magna
	0.1	21d, rpd, Daphnia magna (Slooff & Canton 1983)
	0.18	Daphnia magna
	0.32	rpd, Daphnia magna (Adema 1978)
	0.0018	21d Daphnia magna (Anon. 1986b)
LC50 values to fishes, mg/l	0.2	Salmo gairdneri (Hodson et al. 1984)
	0.136–0.287	96hr, Micropterus salmoides juv. (Johansen et al. 1985)
	0.096	96hr, Salmo gairdneri (Voss et al.1980)
	0.1	24hr, Cyprinus carpio (Hashimoto et al. 1982)
	0.032–0.130	96hr, Notopterus notopterus (Gupta et al. 1982)
	0.47	96hr, Pimephales promelas (Cleveland et al. 1982)
	0.4	48hr, Leuciscus idus (Wellens 1982)
	0.77–0.97	96hr, Poecilia reticulata (Gupta et al. 1982)
	0.11	act, Lepomis macrochirus
	0.052	act, Salmo gairdneri
	0.205	act, Pimephales promelas (Kenaga 1979)
	0.066	4d, Alburnus alburnus
	0.087	2d, Carassius carassius
	0.043	4d, Coregonus muksun
	0.045	4d, Esox lucius
	0.038	4d, Rutilus rutilus
	0.054	4d, Salmo trutta lacustris (Oikari 1987)
	0.066	Dowicide G: 96hr, Lagodon rhomboides (Verschueren 1983)
	0.055	Oncorhynchus kisutch
	0.071	Salmo gairdneri
	0.128	Salvelinus fontinalis
	0.22	Carassius auratus
	0.212	Pimephales promelas
	0.217	Poecilia reticulata
	0.138	Lepomis macrochirus
	0.19	Brachydanio rerio
	0.118	14d, Salvelinus fontinalis
	0.153	14d, Pimephales promelas
	0.188	14d, Lepomis macrochirus (Anon. 1986b)
	0.117	test 1, 96hr, Carassius auratus
	< 0.053	test1, 96hr, Ictalurus punctatus
	0.15	test1, 96hr, Lepomis macrochirus (Phipps & Holcombe 1985)
	0.2	Poecilia, pH7, 48hr (Landner 1969)
	0.04	Poecilia, pH5, 96hr (Saarikoski & Viluksela 81)
	0.48	96hr, Salmo gairdneri, pH5.7 (Davis & Hoos 75)
	0.095	96hr, Pimephales, pH6.5
	0.26	96hr, Pimephales, pH8 (Spehar et al.1985)
	305	48hr, Oryzias latipes (MITI 1992)
EC50 values to fishes, mg/l	0.002	Oncorhynchus, grw (Landner & Skoglund 1977)

PQR

LOEC values to fishes, mg/l	0.025	srv, grw, schr, Salmo gairdneri (Hodson & Blunt 1981)
	0.389	srv, chr, Cyprinodon variegatus (Ward & Parrish 1980)
	0.088	srv, chr, Cyprinodon variegatus (Parrish et al. 1978)
	0.073	grw, schr, Pimephales promelas (Holcombe et al. 1982)
NOEC values to fishes, mg/l	0.01	srv, grw, schr, Salmo gairdneri (Hodson & Blunt 1981)
	0.047	srv, chr, Cyprinodon variegatus (Parrish et al. 1978)
	0.045	grw, schr, Pimephales promelas (Holcombe et al. 1982)
	0.0125	14d, Brachydanio rerio (Anon. 1986b)
	0.0048	14d, Brachydanio rerio (Anon. 1986b)
	0.32	28d, srv, Poecilia reticulata
	0.32	28d, srv + bhv, Poecilia reticulata
	0.1	28d, grw, Poecilia reticulata
	0.032	40d, srv, Oryzias latipes
	0.032	40d, srv + bhv, Oryzias latipes
	0.32	40d, grw, Oryzias latipes (Slooff & Canton 1983)
Effects on the physiology of water organisms	Cyprinus carpio, 0.1 mg/100g/day, 10 d → Gammarus pseudolimnaeus, 1.680 mg/l, 2 d → biochemical effect (change in physiochemical process including glycogen uptake, cholesterol levels and lipid analysis) (Kobayashi et al. 1987).	
	Micropterus salmoides, 0.0252 mg/l, 52 d, measurable change in length and/or weight (Johansen et al. 1987).	
	Salmo gairdneri, 0.020 mg/l, 4 d, change in enzyme activity (Castren & Oikari 1987).	
	Pimephales, srv, grw, 90 days, > 0.14 mg/l (Cleveland et al. 1982).	
Other information about water organisms	EC50 (24hr), 0.15 mg/l, rpd, Tetrahymena pyriformis (Yoshioka et al. 1985).	
	EC50, 2 d, grw, 0.720 mg/l, Tetrahymena pyriformis (Schultz 1987).	
	LC50 (96hr), 0.16–0.19 mg/l, Lymnea acuminata (Gupta & Rao 1982).	
	LOEC 0.6 mg/l, Colpidium campylum (Dive et al. 1980).	
	EC50, 1 d, 631.0–1556.0 mg/l, Chironomus riparius (Fisher 1986).	
	Lethal threshold concentration (LT50): 0.0881 mg/l, 1.32 d, Salmo gairdneri (McKim et al. 1987).	
	NOEC, 0.032 mg/l, 21d, Hydra oligactis, specific growth rate. NOEC, 0.1 mg/l, 40d, Lymnaea stagnalis, mortality. NOEC, 0.01 mg/l, 40d, Lymnaea stagnalis, reproduction. NOEC, 0.0032 mg/l, 40d, Lymnaea stagnalis, hatching. (Slooff & Canton 1983)	
	LC50, 0.157 mg/l, 96hr, test 1, snail. LC50, 0.142 mg/l, 96hr, test 3, snail. (Phipps & Holcombe 1985)	
	LC50, 48hr, 1.0 mg/l, Tubificidae LC50, 48hr, 0.11 mg/l, Chironomus gr. thummi LC50, 48hr, 0.25 mg/l, Erpobdella octoculata LC50, 48hr, 0.56 mg/l, Lymnaea stagnalis LC50, 48hr, 0.13 mg/l, Dugesia cf. lugubris LC50, 48hr, 0.73 mg/l, Hydra oligactis LC50, 48hr, 11 mg/l, Corixa punctata LC50, 48hr, 42 mg/l, Ischura elegans LC50, 48hr, 0.38 mg/l, Nemoura cinerea LC50, 48hr, 5.9 mg/l, Cloeon dipterum (Slooff 1983)	

	Melosira, EC21, 0.001 mg/l (Gotham & Rhee 1982). Crassostrea, embryo, EC50, 48hr, 0.04 mg/l (Borthwick & Schimmel 1978).
Other information	Toxicity decreases when the hardness of water increases (Berglind & Dave 1984). In nature pentachlorophenol is O-methylized to anisole (Allard et al. 1987). Degradation of pentachlorophenol (Murphy et al. 1979): → methyl ether PCP PCP → 2,3,5,6 tetraCP → 2,3,6 triCP → 2,3,4,5 tetraCP Alternative degradation routes for pentachlorophenol (Reinert et al. 1978).

1574 • 1,1,2,3,3-Pentachloropropane 15104-61-7

Sumformula of the chemical	C3H3Cl5
Water solubility, mg/l	410 (MITI 1992)
Melting point, °C	< -10 (MITI 1992)
Boiling point, °C	204 ± 1 (MITI 1992)
Log octanol/water coefficient, log Pow	3.23 (MITI 1992)
Total degradation in water	Biodegradation: 0% by TOC (altered to 1,2,3,3-(or 1,1,3,3-)Tetrachloro-propene period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

1575 • n-Pentadecane 629-62-9

Synonyms	Pentadecane
Sumformula of the chemical	C15H32
EINECS-number	2110981
Melting point, °C	10 (MITI 1992)
Boiling point, °C	270.5 (MITI 1992)
Total degradation in water	Biodegradation: 54.8% by BOD (on the upward trend) period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
Bioconcentration factor, fishes	6.8–20.4 8w, Cyprinus carpio, conc 2 mg/l 13.2–19.7 8w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	1900 48hr, Oryzias latipes (MITI 1992)

PQR

1576 • Pentaerythritol 115-77-5

Synonyms	2,2-Bis(hydroxymethyl)-1,3-propanediol
Sumformula of the chemical	C5H12O4
EINECS-number	2041049
Water solubility, mg/l	71000 (MITI 1992)
Melting point, °C	202 (MITI 1992)
Boiling point, °C	276 30 mmHg (MITI 1992)
Total degradation in water	Biodegradation: 13% by BOD period: 25d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Bioconcentration factor, fishes	0.3–0.6 6w, Cyprinus carpio, conc 10 mg/l 0.4–2.1 6w, Cyprinus carpio, conc 1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	> 50000 48hr, Oryzias latipes (MITI 1992)

1577 • Pentafluorophenol 771-61-9

Other information about water organisms	EC50, grw, 2 d, 4.3 mg/l, Tetrahymena pyriformis (Schultz 1987).

1578 • Pentane 109-66-0

Use	Solvent.
Water solubility, mg/l	40
Boiling point, °C	36.1
Log octanol/water coefficient, log Pow	3.45 (Sangster 1989)
Henry's law constant, Pa x m³/mol	128100 calc. (Yaws et al. 1991)
Volatilization	Relative volatility (nBuAc=1) = 35.77
TCLo values to mammals in inhalation exposure, ppm	13000 CNS eff. – rat

PQR

1579 • 2,4-Pentanedione 123-54-6

Odour	Quality: sour, rancid Hedonic tone: unpleasant Threshold odour concentration absolute: 0.01 ppm 50% recognition: 0.020 ppm 100% recognition: 0.024 ppm Odour index 100% recognition: 384 166 (Hellman & Small 1974).
Water solubility, mg/l	> 100000 (MITI 1992)
Melting point, °C	-23 (MITI 1992)
Boiling point, °C	137–141 (MITI 1992)
Total degradation in water	Biodegradation: 79-88% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 67 mg/l (Bringmann & Kühn 1980a).
EC50 values to microorganism, mg/l	375 Microtox (Nacci et al. 1986)
LOEC values to algae, mg/l	8.5 rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976) 2.7 rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
LC50 values to crustaceans, mg/l	> 217 96hr, Orconectes nais (Phipps & Holcombe 1985)
LC50 values to fishes, mg/l	71.6 96hr, Salmo gairdneri 74.3 96hr, Lepomis macrochirus 155 96hr, Pimephales promelas 107 96hr, Carassius auratus 83.6 96hr, Ictalurus punctatus (Phipps & Holcombe 1985)
Other information about water organisms	LOEC 5.9 mg/l, rpd, schr, Uronema parduczi (Bringmann & Kühn 1980b). LC50, 155 mg/l, 96hr, snail (Phipps & Holcombe 1985). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 2.7 mg/l protozoa (Entosiphon sulcatum): 11 mg/l (Bringmann & Kühn 1980a).

PQR

1580 • 2-Pentanol 6032-29-7

Synonyms	Methylpropylcarbinol 1-Methyl-1-butanol
Sumformula of the chemical	CH3(CH2)2CHOHCH3
Molecular weight	88.15
Specific gravity (water=1)	0.809 at 20/4 °C
Vapour density (air=1)	3.04
Water solubility, mg/l	53000 at 30 °C

Boiling point, °C	119	
Log octanol/water coefficient, log Pow	1.34 1.21	 (Sangster 1989)
Other information about mammals	Mammalia: rabbit: single oral LD50: 4.25 ml/kg (Verschueren 1983).	
EC50 values to microorganism, mg/l	4672	Biodegradation inhibition (Vaishnav 1986)

1581 • 3-Pentanol

584-02-1

Sumformula of the chemical	C5H12O	
Log octanol/water coefficient, log Pow	1.21	(Sangster 1989)
EC50 values to microorganism, mg/l	1500	15 min Microtox (Hermens et al. 1985)
LC50 values to fishes, mg/l	990	7d, Poecilia reticulata, Könemann 1979

1582 • 2-Pentanone

107-87-9

Sumformula of the chemical	C5H10O	
Use	Solvent.	
Boiling point, °C	102	
Log octanol/water coefficient, log Pow	0.84	(Sangster 1989)

1583 • 3-Pentanone

96-22-0

Synonyms	Diethyl ketone Dimethylacetone Propione	
Sumformula of the chemical	C5H10O	
Use	Solvent.	
Molecular weight	86.15	
Boiling point, °C	101.5	
Log octanol/water coefficient, log Pow	0.82	(Sangster 1989)
Chemical oxygen demand, g O2/g	2.31	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g O2/g	1.98	5 days (Bridie et al. 1979)
LD50 values to mammals in oral exposure, mg/kg	8000 2140	orl-rat orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	513	ivn-mus (Lewis & Sweet 1984)
LDLo values to mammals in non-oral exposure, mg/kg	1250	ipr-rat (Lewis & Sweet 1984)

LCLo values to mammals in inhalation exposure, ppm	8000	ihl-rat (Lewis & Sweet 1984)
EC50 values to microorganism, mg/l	7925	Biodegradation inhibition (Vaishnav 1986)
LC50 values to fishes, mg/l	1200	24hr, Carassius auratus (Bridie et al. 1979)

1584 • p-(tert-Pentyl)phenol

80-46-6

Synonyms	4-tert-Amylphenol p-(α, α-Dimethylpropyl)phenol p-(1,1-Dimethylpropyl)phenol 4-(1,1-Dimethylpropyl)phenol	
Sumformula of the chemical	C11H16O	
Molecular weight	164.27	
LD50 values to mammals in oral exposure, mg/kg	1830	orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	2000	skn-rbt (Lewis & Sweet 1984)
LC50 values to fishes, mg/l	2.5	96hr, Pimephales promelas (Holcombe et al. 1984)
Other information about water organisms	Tetrahymena pyriformis; EC50, grw, 2 d, 9.61 mg/l (Schultz 1987).	

1585 • Pentylamine

110-58-7

Sumformula of the chemical	C5H13N	
Synonyms	n-Amylamine	
EINECS-number	2037802	
Molecular weight	87.16	
Water solubility, mg/l	> 1000	(MITI 1992)
Specific gravity (water=1)	0.77	at 20/4 °C
Vapour density (air=1)	3.01	
Conversion factor, 1 ppm in air=	3.56	mg/m³
Conversion factor, 1 mg/m³ in air=	0.281	ppm
Vapour pressure, mmHg	35	at 26 °C
Melting point, °C	-55	
Boiling point, °C	104	
Log octanol/water coefficient, log Pow	1.05	calculated
Total degradation in water	Biodegradation: 72–76% by BOD (on the upward trend) period: 21d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	

PQR

Effects on wastewater treatment	Degradation by Aerobacter: 200 mg/l at 30 °C: parent: 100% in 25 hours mutant: 100% in 9 hours (Verschueren 1983).

1586 • 2-Pentylanthraquinone 13936-21-5

Sumformula of the chemical	C19H18O2
Melting point, °C	23.2–29.8 (MITI 1992)
Total degradation in water	Biodegradation: 7% by BOD period: 14d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).
Bioconcentration factor, fishes	336–2070 8w, Cyprinus carpio, conc 0.135 mg/l 557–1070 8w, Cyprinus carpio, conc 0.0135 mg/l (MITI 1992)
LC50 values to fishes, mg/l	86 48hr, Oryzias latipes (MITI 1992)

1587 • α-Pentylcinnam aldehyde 1331-92-6

Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

1588 • Peracetic acid 79-21-0

Synonyms	Peroxyacetic acid PAA Ethaneperoxoid acid
Sumformula of the chemical	C2H4O3
EINECS-number	2011868
Products containing the chemical	Desirox
Purity, %	5–15 (WPSREG 1994)
Known impurities	water acetic acid (CH3COOH) hydrogenperoxide (H2O2) dinatriumpyrophosphate ammoniumnitrate (WPSREG 1994).
Use	Active substance in slimicides: to prevent slime and clogging caused by harmful micro-organisms in cooling and circulating water systems and paper production (WPSREG 1994).
State and appearance	Colourless liquid (WPSREG 1994).
Molecular weight	76.05
Density, kg/m³	1200 (WPSREG 1994)
Vapour pressure, mmHg	0.0085–0.009 (WPSREG 1994)
Melting point, °C	0.1 (WPSREG 1994)

Boiling point, °C	103 (WPSREG 1994)
Flashing point, °C	> 100 for concentrated solution 40.6 °C (WPSREG 1994)
pKa	8.2
Log octanol/water coefficient, log Pow	-0.924 calculated (WPSREG 1994)
Other physicochemical properties	Completely water soluble. Soluble in alcohol and in ether, com pletely soluble in polar solvents, poorly in aromatic solvents. Henry's law constant 2.08 x 0.000001 atm x m^3/mol (25 °C, experimental). Oxidizing (as over 12% solution), corrosive. (WPSREG 1994).
Other information about degradation	Hydrolysis: 0.2% solution in pH 2.7 nearly stabile; T1/2 (20 °C) about 1 week in pH 4.4 and 1 d in pH 7; < 0.02% PAA-solution T1/2 = about 24hr (pH not known). (WPSREG 1994).
Other information about bioaccumulation	Not bioaccumulative (WPSREG 1994).
LD50 values to mammals in oral exposure, mg/kg	23–330 orl rat, calculated (WPSREG 1994)
Effects on wastewater treatment	NOEC for microbs in the active sludge 25–50 mg/l (WPSREG 1994).
EC50 values to algae, mg/l	≥ 0.7 (absorbance, 96hr), Anabaena variabilis ≥ 1.6 (absorbance, 96hr), Synecococcus leopoliensis ≥ 12 (absorbance, 72hr), Chlamydomonas eugametos ≥ 4.0 (absorbance, 96hr), Scenedesmus quadricauda (WPSREG 1994)
LOEC values to algae, mg/l	≥ 1.1 (growth, 96hr), Anabaena variabilis ≥ 2.3 (growth, 96hr), Synecococcus leopoliensis ≥ 17 (growth, 72hr), Chlamydomonas eugametos ≥ 16 (growth, 96hr), Scenedesmus quadricauda (WPSREG 1994)
EC50 values to crustaceans, mg/l	108–149 product, 12% PAA, 96hr, Crangon crangon (sea water) 1.75–2.55 product, 12% PAA, 48hr, larvaes of Mytilus edulis (sea water) 2.10–2.40 product, 12% PAA, 48hr, larvaes of Crassotrea gigas (sea water) (WPSREG 1994)
LC50 values to fishes, mg/l	10–18 product, 12% PAA, Salmo gairdneri 80–99 product, 12% PAA, Pleuronectes platessa (sea water) (WPSREG 1994)
Other information	LC99.9 = 1-150 mg/l, Escherichia coli LC99.9 = 6-1000 mg/l, Streptococcus faecalis (influence depends on the properties of the test solution) NOEC = 25-50 mg/l, active sludge microbs (WPSREG 1994).

1589 • Perfluidone 37924-13-3

Use	Herbicide.
Effects on plants	Tubers of Cyperus rotundus L. were planted to soil sprayed with 1 kg perfluidone/ha → a decrease in number of nutsedge (C. rotundus) sprouts above ground (6 weeks after treatment) (Rincon & Warren 1979).

PQR

1590 • Perfluorotributylamine

311-89-7

Sumformula of the chemical	C12NF27
Water solubility, mg/l	< 10 (MITI 1992)
Boiling point, °C	177–178 (MITI 1992)
Log octanol/water coefficient, log Pow	2.69 (MITI 1992)
Total degradation in water	Biodegradation: 0–10% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	3.3–8.8 6w, Cyprinus carpio, conc 0.1 mg/l 19–34 6w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	> 500 48hr, Oryzias latipes, MITI 1992

1591 • Permethrin

52645-53-1

Synonyms	3-Phenoxybenzyl-cis, trans-3-(2,2-dichlorovinyl)-2,2-dimethyl-cyclopropanecarboxylate
Sumformula of the chemical	C21H20Cl2O3
Products containing the chemical	Ambush
Use	Active ingredient in insecticides.
Molecular weight	391.31
Vapour pressure, mmHg	0.000000018 mmHg (KEMI 1990)
Water solubility, mg/l	0.04 room temperature 0.2 at 20 °C (KEMI 1990)
Melting point, °C	63–65 (KEMI 1990)
Log octanol/water coefficient, log Pow	6.5 at 25 °C (KEMI 1990)
Mobility	Permethrin is bound very tightly to soil and it can be kept almost immobile. Trans-isomer and some of degradation products are bound lighter than cis-isomer. Koc: 14000 for permethrin and Koc: 70–350 for degradation products (KEMI 1990).
Photochemical degradation in air	Permethrin is degraded for instance from surfaces of leaves very slowly because of slow photolysis.
Hydrolysis in water	About 90% of permethrin has been hydrolyzed at pH 7 during 30–40 days. At higher pH it will hydrolyzed quicklier. Cis-isomer is more stabile against photolysis and hydrolysis than trans-isomer. (KEMI 1990)
Degradation and transformation products	cis/trans-3-(2,2-diclorovinyl)-2,2-dimethylcyclopropane-carboxylate; 3-phenoxybenzylalcohol; 3-phenoxybenzoate. (KEMI 1990)

Other information about degradation	Permethrin degrades in soil and water by influence of microorganisms. The half-life for primary degradation in soil is 5–12 days at 25 °C and 14–55 days at 10 °C. Degradation is prevented in soil, if it contains high amount organic material. In natural water degradation is prevented, because permethrin is bounded to particles and sediment. (KEMI 1990)
Bioconcentration factor, fishes	55 Salmo salax (Verschueren 1983)
Bioconcentration factor, crustaceans	800–2400 blue-green algae (KEMI 1990)
LD50 values to mammals in oral exposure, mg/kg	410 orl-rat (Lewis & Sweet 1984) 500–4000 orl-rat, orl-mus, orl-gpg, orl-rbt (KEMI 1990)
LD50 values to mammals in non-oral exposure, mg/kg	> 4000 idr-rat, idr-rbt (KEMI 1990)
LC50 values to mammals in inhalation exposure, mg/m³	> 23.5 mg/l, ihl-rat (KEMI 1990)
LD50 values to birds in oral exposure, mg/kg	> 3500 mg/kg, body weight (KEMI 1990)
Subacute LC50 values to birds in feeding exposure, mg/kg	> 10000 mg/kg, 8d, feed (KEMI 1990)
Effects on amphibia	LD50, 0.14–7.5 mg/kg, Rana pipiens. (KEMI 1990)
Effects on invertebrates	LC50, 2 d: 0.0074 mg/l, Ophiogomphus sp.; 0.0032 mg/l, Pycnopsyche sp.; 0.0045 mg/l, Simulium venustum (Poirier & Surgeoner 1987). Invertebrates, 8.8 g/ha, 1 d, change in species diversity (Kreutzweiser & Kingsbury 1987).
Effects on bees	LD50, 24hr, 0.19–0.28 µg/bee. (KEMI 1990)
Effects on arthropods	Aedes aegypti, LC50, 3 d, 0.00152 mg/l (Helson et al. 1986). Insecta: 8.8 g/ha, 0.5 d, changes in number of larval aquatic insects to travel a given distance in a stream (Kreutzweiser & Kingsbury 1987).
EC50 values to algae, mg/l	1.6–5 mg permethrin/l, Anabaena inaequalis (KEMI 1990)
LC50 values to crustaceans, mg/l	0.0002–0.0006 48hr, Daphnia magna (Stratton & Corke 1981) 0.00014 96hr, Crangon sepstemspiosa 0.00073 96hr, Homarus americanus (McLeese et al. 1980) 0.00025–0.00037 2d Gammarus pseudolimnaeus (Helson et al. 1986)
EC50 values to crustaceans, mg/l	0.0001–0.0002 48hr, Daphnia magna (KEMI 1990)
NOEC values to crustaceans, mg/l	0.1 23d, rpd, Daphnia magna (KEMI 1990)

LC50 values to fishes, mg/l	0.0025	96hr, Salmo gairdneri (Nikunen et al. 1986)
	0.006	48hr, Salmo gairdneri (Mulla et al. 1978)
	0.009	48hr, Salmo salar (Zitko et al.1977)
	0.016	96hr, Pimephales promelas
	0.007	96hr, Salmo gairdneri (Holcombe et al. 1982)
	0.0011	96hr, Ictalurus punctatus
	0.015	96hr, Gambusia affinis (Jolly et al. 1978)
	0.0012	96hr, Salmo salar (McLeese et al.1980)
	0.009	96hr, Salmo gairdneri (Pesticide Manual 1983)
LOEC values to fishes, mg/l	0.0014	srv, schr, Pimephales promelas (Spehar et al. 1983)
NOEC values to fishes, mg/l	0.007	srv, schr, Pimephales promelas (Spehar et al. 1983)
Effects on the physiology of water organisms	Salmo gairdneri, 0.00065 mg/l, 42 d, measurable change in length and/or weight (Kumaraguru & Beamish 1986).	
Other information about water organisms	LC50 (6hr), 0.0006–0.0021 mg/l, Hexagenia rigida (Friesen et al. 1983). Permethrin has in general low acute toxicity to green algae and blue-green algae, expect the blue-green algae Anabaena inaequalis. Degradationproducts 3-phenoxybenzaldehyde and 3-phenoxybenzylalcohol have without exception little higher toxicity for algae than permethrin. (KEMI 1990).	

1592 • Permethrin (cis-isomer) 54774-45-7

LC50 values to fishes, mg/l	0.025	24hr, Salmo gairdneri (Glickman et al. 1981)

1593 • Permethrin (trans-isomer) 51877-74-8

LC50 values to fishes, mg/l	0.014	24hr, Salmo gairdneri (Glickman et al. 1981)

1594 • Peroxyacetylnitrate 2278-22-0

Synonyms	PAN	
Molecular weight	121.06	
Effects on plants	Laboratory evidence with agricultural species indicate a sensitive plant threshold dose of approximately 0.01–0.02 ppm (0.049–0.099 mg/m³) for 4 hours (U.S. Environmental Protection Agency 1976).	
LC50 values to mammals in inhalation exposure, ppm:	106	2hr, ihl-mus (Lewis & Sweet 1984)
	95	0.48 mg/l, 4hr, ihl-rat (Lewis & Sweet 1984)

1595 • Perylene 198-55-0

Sumformula of the chemical	C20H12	
Log octanol/water coefficient, log Pow	6.25	(Sangster 1989)
Other information about water organisms	Lethal threshold concentration (LT50): 0.76 d, 0.0006 mg/l (Newsted & Giesy 1987).	

PQR

1596 • Phenanthrene 85-01-8

Sumformula of the chemical	C14H10
Melting point, °C	101 (MITI 1992)
Boiling point, °C	339 (MITI 1992)
Log octanol/water coefficient, log Pow	4.5 (Anon. 1986) 4.46 observed (Chin et al. 1986) 4.46 (Mackay 1982) 4.52 (Sangster 1989)
Total degradation in water	Biodegradation: 54.0% by BOD (on the upward trend) period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
Other information about degradation	Degradation of phenanthrene:

ENVIRONMENT	INIT.CONC. mg/l	REDOX COND.	TEMP. °C	DEGRADATION %/day	REF.
water	5	aerobic	25	100/7	a
water	10	aerobic	25	100/7	a
freshwater	1	aerobic	5	0/28	b
freshwater	1	aerobic	15	10/28	b
freshwater	1	aerobic	20	37/28	b
freshwater	0.1	aerobic	25	60/28	b
freshwater	1	aerobic	25	47/28	b
freshwater	1	aerobic	37	89/28	b
freshwater	1	aerobic	45	0/28	b
groundwater	0.20	aerobic	10–13	100/2	c
groundwater	0.65	aerobic	10–13	100/2	c
groundwater	0.65	aerobic	10–13	90/4	c
soil	2.1	aerobic	–	27/10	d
soil	25.00	aerobic	–	83/3	e

a) Tabak et al. 1981
b) Sherrill & Sayler 1980
c) Jensen et al. 1985
d) Sisler & Zobell 1974
e) Groenewegen & Stolp 1976
(Anon. 1987b).

LD50 values to birds in oral exposure, mg/kg	> 113 orl-Agelaius phoeniceus (Schafer et al. 1983)
LC50 values to crustaceans, mg/l	0.1 96hr, Daphnia pulex (Trucco et al. 1983)
EC50 values to crustaceans, mg/l	0.734 2d, Daphnia pulex (Passino & Smith 1987)
LC50 values to fishes, mg/l	0.04 0d, embryo-larval, Salmo gairdneri 0.04 4d, embryo-larval, Salmo gairdneri > 0.07 0d, embryo-larval, Micropterus salmoides 0.18 4d, embryo-larval, Micropterus salmoides (Black et al. 1983)

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1597 • Phenanthrene quinone 84-11-7

LD50 values to birds in oral exposure, mg/kg	> 104	orl-Agelaius phoeniceus (Schafer et al. 1983)
EC50 values to algae, mg/l	0.38	grw, act, 72hr, Dunaliella bioculata (Heldal et al. 1984)

1598 • Phenazin-5-oxide 304-81-4

EC50 values to algae, mg/l	0.9	rpd, act, Chlamydomonas reinhardii (Lee & Hong 1982)

1599 • Phenetole 103-73-1

Sumformula of the chemical	C8H10O	
Water solubility, mg/l	100	(MITI 1992)
Melting point, °C	-33	(MITI 1992)
Boiling point, °C	172	(MITI 1992)
Total degradation in water	Biodegradation: 63% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

1600 • Phenmedipham 13684-63-4

Sumformula of the chemical	C16H16N2O4	
Use	Active ingredient in herbicides.	
Vapour pressure, mmHg	0.00000007, 25 °C (KEMI 1990)	
Water solubility, mg/l	4.7	at 20 °C (KEMI 1990)
Melting point, °C	143–144	(KEMI 1990)
Log octanol/water coefficient, log Pow	3.5	(KEMI 1990)
Mobility	Phenmedipham was bound tightly to soil. In a soil (sandy loam) column study 95% was retained in the upper 5 cm. In the studies on thin-layer plates phenmedipham was found to have low mobility The major hydrolyse product methyl-3-hydroxyphenylcarbamate (MHPC) was more mobile. Rf < 0.1; Koc 500–750 for phenmedipham (KEMI 1990).	
Photochemical degradation in soil	The photolysis half-life of phenmedipham on soil surface is about 3 days (KEMI 1990).	
Hydrolysis in water	Phenmedipham is hydrolysed very quickly to methyl-3-hydroxyphenylcarbamate (MHPC). It is hydrolysed quickiest under the basic conditions, the half-life is 72 min at pH 9 (KEMI 1991).	
Degradation and transformation products	Methyl-3-hydroxyphenylcarbamate (MHPC) (KEMI 1990).	
Other information about degradation	Degradation of phenmedipham is depending on pH. The half-life for the primary biological degradation in soil has been found to be 20–120 days under aerobic conditions. The longer time is observed in acid soil. Methyl-3-hydroxyphenylcarbamate (MHPC) degrades more quickly; half-life is 20–30 days. The complite degradation of phenmedipham happens however very slowly, the half-life is 700–800 days (KEMI 1990).	

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Other information about bioaccumulation	BCF: 165 (in whole fish) (KEMI 1990).	
LD50 values to mammals in oral exposure, mg/kg	> 3000 1520	oral-rat, mus, gpg (KEMI 1990) transf.pr. MHPC, oral-rat (KEMI 1990)
LD50 values to mammals in non-oral exposure, mg/kg	> 4000	mg/kg, idr-rat (KEMI 1990)
LD50 values to birds in oral exposure, mg/kg	> 2500	quail, duck (KEMI 1990)
Subacute LC50 values to birds in feeding exposure, mg/kg	10000	0000, 8d, feed, quail, duck (KEMI 1990)
Effects on reptiles	LC50, earthworm, 156 mg/kg soil, 14d (KEMI 1990).	
Effects on bees	LC50, 96hr, 4100 µg/bee (oral) (KEMI 1990).	
Effects on plants	1.0 kg phenmediphan /ha was applied with a sprayer 24 days after seeding to lamb's-quarters (Chenopodium album L.) in the 3- to 4-leaf stage → decrease in shoot growth and plant number (Jensen et al. 1977).	
Effects on microorganisms	Phenmedpham has no effect on the nitrification or ammonification in soil with recommended dose. NOEC (28d): 1.3mg/kg soil (KEMI 1990).	
EC50 values to algae, mg/l	0.13	96hr, grw, Scenedesmus (KEMI 1990)
NOEC values to algae, mg/l	0.008	96hr, Scenedesmus (KEMI 1990)
EC50 values to crustaceans, mg/l	0.5	24hr, mbt, Daphnia magna (KEMI 1990)
LC50 values to fishes, mg/l	1.4–4	mg/l, 96hr, different kind of fishes (KEMI 1991)
LOEC values to fishes, mg/l	1.6 2.4	Salmo gairdneri Cyprinus carpio (Pesticide Manual 1983)
NOEC values to fishes, mg/l	1	96hr (KEMI 1990)

1601 • Phenobarbital

50-06-6

Synonyms	Phenylbarbital Phenylethylmalonylurea 5-Ethyl-5-phenylbarbituric acid	
Sumformula of the chemical	C12H12N2O3	
Use	Medicine (sedative), laboratory reagent. Also available as the sodium salt which has good water-solubility.	
State and appearance	White, shining, crystalline powder, stable.	
Odour	Odourless.	
Melting point, °C	174–178 °C	
Log octanol/water coefficient, log Pow	1.28	(Anon. 1986)
Other physicochemical properties	Soluble in alcohol, ether, chloroform, alkali hydroxides, alkali carbonate solutions; sparingly soluble in water.	
LD50 values to birds in oral exposure, mg/kg	> 100	orl-Agelaius phoeniceus (Schafer et al. 1983)

PQR

1602 • Phenol

108-95-2

Synonyms	Hydroxybenzene Phenylic acid Carbolic acid Monohydroxybenzene Oxybenzene Phenic acid Phenyl hydrate Benzenol Monophenol Phenol alcohol Phenyl hydroxide Phenylic alcohol	
Sumformula of the chemical	C6H6O	
Use	Solvent. Produced by cumene oxidation and is used as an intermediate in the manufacture of a wide range of important chemicals including phenolic resins, bisphenol-A, caprolactam, alkylphenols and adipic acid. Disinfectant.	
State and appearance	Colourless till brown-black.	
Odour	Threshold odour concentration in water: 1.0–7.5 mg/l (Fawell & Hunt 1988). Odour: characteristic, medicinal, sickening sweet and acrid with a sharp and burning taste (Verschueren 1983). Human odour perception: human reflex response: animal chronic exposure:	 non perception: 0.022 mg/m³; perception: 0.184 mg/m³; adverse response: 0.015 mg/m³; no effect: 0.01 mg/m³; adverse effect: 0.1 mg/m³ (Verschueren 1983).
	Odour index: 16 at 20 °C (Verschueren 1983).	
Molecular weight	94.12	
Specific gravity (water=1)	1.07	
Vapour density (air=1)	3.24	
Conversion factor, 1 ppm in air=	3.92	mg/m³
Conversion factor, 1 mg/m³ in air=	0.26	ppm
Vapour pressure, mmHg	0.2 1 0.524	20 °C 40 °C 25 °C (Daubert & Danner 1985)
Water solubility, mg/l	82000 86600 87000	15 °C 20 °C 25 °C (Howard I 1990) sol (MITI 1992)
Melting point, °C	43 40.9	(Howard I 1990) (MITI 1992)
Boiling point, °C	182 181.75 181.8	at 760 mmHg at 760 mmHg (Howard I 1990) (MITI 1992)
pKa	9.994	(Serjeant & Dempsey 1979)

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Log octanol/water coefficient, log Pow	1.46 (Chin et al. 1986) 1.5 (Anon. 1986) 1.5 (Anon. 1988) 1.46 (Hansch & Leo 1985) 1.5 (Sangster 1989)
Henry's law constant, Pa x m³/mol	0.031 (Anon. 1988) 0.04 (Hine & Mokerjee 1975)
Volatilization	Despite its moderate vapour pressure, phenol has a low Henry's Law constant and a low rate of evaporation from water. The estimated half-life for evaporation from water is 3.2 months. (Branson 1978, Shen 1982) Using the Henry's Law constant, a half-life of 88 days was calculated for evaporation from a model river 1 m deep with a current of 3 m/sec and with a wind velocity of 3 m/sec. (Lyman et al. 1982) Volatilization from near-surface soil should be relatively rapid due to its moderate vapour pressure. (Howard I 1990)
Adsorption/desorption	Low absorptivity to clay soils and silt loam is reported. (Artiola-Fortuny & Fuller 1982) Koc values for two silt loams are 39 and 91. (Scott et al. 1983) No adsorption to aquifer material was observed. (Ehrlich et al. 1982) Using the log Kow, an estimated Koc of 148 was calculated. (Lyman et al. 1982)
Mobility	2.83% (air), 96.17% (water), 1.00% (sediment). Equilibrium distribution: *mass%* air 1.05 water 98.47 solid 0.48 (Anon. 1988). Based on the reported and estimated Koc, phenol will be expected to exhibit high to very high mobility in soil. (Swann et al. 1983)
Photochemical degradation in air	Phenol absorbs light in region 290–330 nm and therefore might directly photo degrade. (Howard I 1990) Phenol's estimated half-life by reaction with hydroxyl radicals in air is 0.61 days. (Hendry & Kenley 1979)
Photochemical degradation in water	Photo oxidation by UV-light in aqueous medium at 50 °C: 10.96% degradation to CO2 after 24hr (Verschueren 1983). Natural sunlight causes degradation in water. (Callahan 1979) Phenol has also been shown to inhibit oxidant formation both in air and in water. (Gitchell et al. 1974) (Draper & Crosby 1983) The estimated half-life for reaction of phenol with photochemically produced singlet oxygen in surface waters contaminated by humic substances is 83 days. (Scull & Hoigne 1987) As a class, phenols react relatively rapidly in sunlit natural water via reaction with photochemically produced hydroxyl radicals and peroxy radicals; typical half-lives for hydroxyl and peroxyl radical reactions are on the order of 100 and 19.2hr of sunlight, respectively. (Mill & Mabey 1985)
Chemical oxygen demand, g 02/g	2.33 5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	1.68 5 days (Bridie et al. 1979)

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Aerobic degradation in soil	AEROBIC DEGRADATION IN SOIL Maximum adsorption wavelength: 271 nm NON-STERILE SOIL Minimum time for > 70% decrease: 0.50–1.00 d % decomposition at the termination of the experiment: 5d, 100% STERILE SOIL % decomposition at the termination of the experiment: 40d, 15% (Baker et al. 1980) Percent mineralization in an alkaline, para-brown soil under aerobic conditions was 45.5%, 48% and 65% after 3,7 and 70 days, respectively. (Haider et al. 1974)
Anaerobic degradation in soil	ANAEROBIC DEGRADATION IN SOIL Maximum adsorption wavelength: 271 nm NON-STERILE SOIL % decomposition at the termination of the experiment: 40d, 20% STERILE SOIL % decomposition at the termination of the experiment: 40d, 7% (Baker et al. 1980)
Aerobic degradation in water	Biodegradation to CO2 in estuarine water: *conc. µg/l* — *month* — *incubation time (hr)* — *degradation rate (µg/l/day) x 1000* — *turnover time (days)* 5 — January — 24 — 270 — 18 10 — January — 24 — 550 — 18 5 — March — 24 — 100 — 25 10 — June — 24 — 580 — 17 (Verschueren 1983).
Total degradation in soil	Decomposition rate in soil suspension: 2 days for complete disappearance (Verschueren 1983). Degradation in soil is completed in 2–5 days even in subsurface soils. (Baker & Mayfield 1980) Half-lives for degradation of low concn of phenol in 2 silt loam soils were 2.70 and 3.51hr. (Scott et al. 1983)
Total degradation in water	Complete degradation in < 1 day in water from 3 lakes; rates increace with increase concn phenol and increase tropic levels of water; rate affected by concn of organic and inorganic nutrients. (Rubin & Alexander 1983) Complete removal in river water after 2 days at 20 °C and after 4 days at 4 °C. (Ludzack & Ettinger 1960) Degradation is somewhat slower in salt water and a half-life of 9 days has been reported in an estuarine river. (Lee & Ryan 1979) Biodegradation: 85% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992)
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

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Other information about degradation

Impact on biodegradation processes:
inhibition of degradation of glucose by Pseudomonas fluorescent: 70 mg/l; inhibition of degradation of glucose by Escherichia coli: > 1000 mg/l; inhibition of the nitrification process in non adapted activated sludge from 5.6 mg/l upwards (Verschueren 1983).

Inhibition of cellulose degradation by natural soil populations	*at 17hr*	*at 200hr*
500 ppm phenol	72%	44.0%
1000 ppm phenol	97.6%	56.5%
1500 ppm phenol	98.4%	60.3%
5000 ppm phenol	98.7%	99.5%

inhibition of starch degradation by natural soil populations	*at 20hr*	*at 140hr*
500 ppm phenol	41%	40.3%
1000 ppm phenol	96%	52.7%
1500 ppm phenol	97.4%	85.1%
5000 ppm phenol	98.4%	98.4%

(Verschueren 1983).

ENVIRONMENT	*INIT.CONC. mg/l*	*REDOX-COND.*	*TEMP. °C*	*DEGRADATION %/day*	*REF.*
water	20	aerobic	25	99/7	a
water	5	aerobic	25	96/7	b
water	10	aerobic	25	97/7	b
water (adapted)	5	aerobic	25	100/7	b
water	0.0001–0.001	aerobic	29	80/10	c
groundwater	30–50	sulfate reducing	room	99/90	d
groundwater	30–50	methanogen	room	100/90	d
lake sediment	30–50	anaerobic	room	100/90	d
activated sludge	30–50	anaerobic	room	100/90	d
activated sludge appr.	50	anaerobic	35	91/14	e
soil suspension	10–100	aerobic	30	100/2	f
soil suspension	25	aerobic	25	100/1	g
soil	1	aerobic	23	100/5	h
soil	1	anaerobic	23	20/40	h
sterile soil	1	aerobic	23	15/40	h
sterile soil	1	anaerobic	23	7/40	h
soil	258	aerobic	20	> 99/3	i

a) Bunch & Chamber 1967
b) Tabak et al. 1981
c) Subba-Rao et al. 1982
d) Gibson & Suflita 1986
e) Horowitz et al. 1982
f) Alexander & Aleem 1961
g) Alexander & Lustigman 1966
h) Baker & Mayfield 1980
i) Lökke 1984 (Anon. 1987b).

Metabolism in mammals

Phenol is readily absorbed by all routes, though it is rapidly conjugated with either sulfate or glucuronic acid, followed by elimination in the urine. Small quantities of oxidative metabolites such as catechol, hydroquinone and benzoquinones can be formed. Such metabolites have been suggested to be involved in the hematotoxicity of benzene, though phenol does appear to have much weaker activity than benzene in this respect (Fawell & Hunt 1988).

Bioconcentration factor, fishes

1.9	Carassius auratus (Freitag et al. 1984)
20	Leuciscus idus melanotus (Freitag et al. 1984)

Bioconcentration factor, crustaceans

277	Daphnia magna (Dauble et al. 1981)

Bioconcentration factor, algae	200 3.5	Chlorella fusca (Freitag et al. 1984) Scenedesmus quadricauda (Hardy et al. 1985)
LD50 values to mammals in oral exposure, mg/kg	384 282 270	orl-rat orl-mus (Lewis & Sweet 1984) orl-mus (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	180 127 112 344 669 850	ipr-mus ipr-rat ivn-mus scu-mus skn-rat skn-rbt (Sweet 1987)
LC50 values to mammals in inhalation exposure, mg/m³	74 177 316	ihl-mam (Lewis & Sweet 1984) ihl-mus ihl-rat (Sweet 1987)
LDLo values to mammals in oral exposure, mg/kg	80 500 14000 140 10 420	orl-cat (Lewis & Sweet 1984) orl-dog orl-hmn orl-hmn orl-infant orl-rbt (Sweet 1987)
LDLo values to mammals in non-oral exposure, mg/kg	300 620 180 500 2000 300 80 450 650	ipr-gpg ipr-rbt ivn-rbt par-cat par-dog par-rbt scu-cat scu-gpg scu-rat (Sweet 1987)
TDLo values to mammals in oral exposure, mg/kg	2300 2600 4000 2800 300 1200	orl-mus, 6-15d preg. effects on fertility effects on embryo or fetus orl-mus, 6-15d preg. effects on embryo or fetus orl-mus, 6-15d preg. specific developmental abnormalities orl-mus, 6-15d preg. effects on embryo or fetus specific developmental abnormalities orl-rat, 6-15d preg. effects on fertility orl-rat, 6-15d preg. effects on embryo or fetus (Sweet 1987)
TDLo values to mammals in non-oral exposure, mg/kg	600	ipr-rat, 12-14d preg. effects on embryo or fetus (Sweet 1987)

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Other information about mammals	Skin and eye irritation data: skin, rabbit, 500 mg, 24hr, severe; skin, rabbit, 535 mg open, severe; skin, rabbit, 100 mg, mild; eye, rabbit, 5 mg, severe; eye, rabbit, 100 mg rinse, mild (Sweet 1987).
Health effects	Man: oral, ingestion, 1000 mg dose may be lethal (Verschueren 1983).
Carcinogenicity	NCI carcinogenesis bioassay completed: results negative; mus, rat (Lewis & Sweet 1984). NCI carcinogenesis bioassay (oral); no evidence; mouse, rat (Sweet 1987).
Mutagenicity	Does not appear to be mutagenic in the Ames test, but has given positive results in some higher test systems (Fawell & Hunt 1988). Mutation data: cyt, fish, multiple, 300 nl/l; dnd, mam, lym, 250 mmol/l; DNA inhibition: hmn, fbr, 10 mmol/l; hmn, hla, 1 mmol/l; mus, orl, 20000 mg/kg; mus, lym, 0.8 mmol/l; dns, rat, orl, 4000 mg/kg; mma, sat, 0.040 mmol/plate; sin, smg, ovr, 100 ppm; sce, hmn, lym, 0.005 mmol/l (Sweet 1987).
LD50 values to birds in oral exposure, mg/kg	> 113 orl-Agelaius phoeniceus (Schafer et al. 1983)
Effects on amphibia	LDLo, 290 mg/kg, par, frog; LDLo, 75 mg/kg, scu, frog; LDLo, 290 mg/kg, scu, frog (Sweet 1987).
Effects on arthropods	Tanytarsus dissimilis, > 51.1 mg/l, LC50, 2 d (Holcombe et al. 1987).
Maximum longterm immission concentration in air for plants, mg/m³	0.2 VDI 2306
Maximum longterm immission concentration in air for plants, ppm	0.05 VDI 2306
Effects on microorganisms	Escherichia coli: > 1000 mg/l (Verschueren 1983). Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 64 mg/l (Bringmann & Kühn 1980a)
EC50 values to microorganism, mg/l	30 Microtox (Beaubien et al. 1986) 2820 Microcalorimetry (Beaubien et al. 1986) 800 OECD 209 (Klecka et al. 1985) 1200 Oxygen uptake (Slabbert and Grabow 1986) 15.1 6hr Growth P. putida (Slabbert 1986) 411 DIDHA (Bitton et al. 1986) 1531 INT (Dutton et al. 1986)
EC50 values to algae, mg/l	290 4hr, Selenastrum capricornutum (Millemann et al. 1984)
LOEC values to algae, mg/l	4.6 Microcystis aeruginosa (Bringmann & Kühn 1980a)

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LC50 values to crustaceans, mg/l	7	50hr, Daphnia magna (Price et al. 1974)
	23	48hr, Daphnia magna (Hermens et al.1984)
	7.7	48hr, Daphnia magna (Lewis 1983)
	40–51	96hr, Gammarus pulex (Stephenson 1983)
	25	96hr, Crangon crangon (Verschueren 1983)
EC50 values to crustaceans, mg/l	10	16d, rpd, Daphnia magna (Hermens et al. 1984)
	12.6	2d, mbt, Daphnia magna (Holcombe et al. 1987)
LC50 values to fishes, mg/l	32 0.15	juv.,96hr, Pimephales promelas juv.,96hr, Salmo gairdneri (Black et al. 1982)
	9.69	act, Salmo gairdneri (Hodson et al.1984)
	7.8	96hr, Salmo gairdneri (Voss et al. 1980)
	13.5 5	96hr, Lepomis macrochirus (Patrick et al. 1968) 24hr, eggs, Salmo gairdneri (Anon. 1973a)
	5.7	96hr, Lepomis macrochirus (Jones 1971)
	8.1–14.0	96hr, 96hr, Notopterus notopterus (Gupta et al.1982)
	46	24hr, Carassius auratus (Bridie et al. 1979)
	10.6 17.4 25.3 10.5	4d, Catostomus commersoni 4d, Lepomis macrochirus 4d, Pimephales promelas 4d, Salmo gairdneri (Holcombe et al. 1987)
	9 11.6 36.3 46	96hr, Gobius minutus 96hr, Branchydanio rerio 96hr, Jordanella floridae 48hr, Ophiocephalus punctatus (Verschueren 1983)
	0.15 0.15 > 5.37 2.8	0d, embryo-larval, Salmo gairdneri 4d, embryo-larval, Salmo gairdneri 0d, embryo-larval, Micropterus salmoides 4d, embryo-larval, Micropterus salmoides (Black et al. 1983)
LOEC values to fishes, mg/l	0.2 2.5	grw, schr, Salmo gairdneri grw, schr, Pimephales promelas (Degraeve et al. 1980)
	3.57	grw, schr, Pimephales promelas (Holcombe et al. 1982)
NOEC values to fishes, mg/l	0.75	grw, schr, Pimephales promelas (DeGraeve et al. 1980)
	1.83	grw, schr, Pimephales promelas (Holcombe et al. 1982)
Effects on the physiology of water organisms	Inhibition of photosynthesis of a freshwater, non-axenic unialgal culture of Selenastrum capricornutum: at 10 mg/l: 105% carbon-14 fixation (vs. controls); 100 mg/l: 92%; 1000 mg/l: 19% (Verschueren 1983).	

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Other information about water organisms	LC50, 96hr, 128.8 mg/l, Lymnea acuminata (Gupta & Rao 1982). LC50, 4d, > 51.1 mg/l, Aplexa hypnorum (Holcombe et al. 1987). Branchydanio rerio, 4.9 mg/l, 27 d, 100% mortality including algicidal and herbicidal effects (Razani et al. 1986). Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 64 mg/l; algae (Microcystis aeruginosa): 4.6 mg/l; green algae (Scenedesmus quadricauda): 7.5 mg/l; protozoa (Entosiphon sulcatum): 33 mg/l; protozoa (Uronema parduczi): 144 mg/l (Verschueren 1983). Chlorella pyrenoidosa, toxic, 233 mg/l (Verschueren 1983). Lethal concentration: rainbow trout: 5 mg/l, 3hr; perch: 9 mg/l, 1hr goldfish: 28.9 mg/l, 48hr (Verschueren 1983). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 7.5 mg/l protozoa (Entosiphon sulcatum): 33 mg/l (Bringmann & Kühn 1980a)
Other information	Reduction of amenities: taste and odour of fish is affected at: 15–25 mg/l; tainting of the flesh of fish and other aquatic organisms: 1–10 mg/l; taste in trout and carp: 25 mg/l; 1.0 mg/l; odour threshold: average: 5.9 ppm; ange: 0.016–16.7 ppm; taste and odour threshold: (tentative): 0.15 mg/l; organoleptic limit: 0.001 mg/l (Verschueren 1983).

1603 • Phenothiazine

92-84-2

Sumformula of the chemical	C12H9NS	
EINECS-number	2021965	
Water solubility, mg/l	< 10	(MITI 1992)
Melting point, °C	182	(MITI 1992)
Boiling point, °C	371	(MITI 1992)
Log octanol/water coefficient, log Pow	3.25	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	127–660 180–528	8w, Cyprinus carpio, conc 0.02 mg/l 8w, Cyprinus carpio, conc 0.002 mg/l (MITI 1992)
LC50 values to fishes, mg/l	1.1	48hr, Oryzias latipes (MITI 1992)

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1604 • Phenoxyacetic acid 122-59-8

Sumformula of the chemical	C8H8O3
Use	Intermediate for dyes, pharmaceuticals, pesticides, other organics, fungicides, flavoring, laboratory reagent, precursor in antibiotic fermentations, especially penicillin V.
State and appearance	Light tan powder.
Melting point, °C	98
Boiling point, °C	285
Log octanol/water coefficient, log Pow	1.41 (Anon. 1986)

1605 • Phenyl benzoate 93-99-2

Synonyms	Benzoic acid, phenyl ester
Sumformula of the chemical	C13H10O2
Log octanol/water coefficient, log Pow	3.59 (Anon. 1986) 3.59 (Sangster 1989)

1606 • 2-Phenyl phenol 90-43-7

Synonyms	2-Hydroxybiphenyl o-Phenylphenol
Sumformula of the chemical	C12H10O
Use	Fungicide.
Molecular weight	170.22
Water solubility, mg/l	30 (MITI 1992)
Melting point, °C	59 (MITI 1992)
Boiling point, °C	275 (MITI 1992)
Total degradation in water	Biodegradation: 47–86% by BOD (on the upward trend) period: 14 d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	2700 orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	50 ipr-mus (Lewis & Sweet 1984)
LDLo values to mammals in oral exposure, mg/kg	15600 orl-mus (Lewis & Sweet 1984)
EC50 values to microorganism, mg/l	30–126 3hr Act. sludge respiration (King and Painter 1986) 56 OECD 209 (Klecka et al. 1985)
LC50 values to fishes, mg/l	5.99 96hr, Pimephales promelas (Holcombe et al. 1984)
Other information about water organisms	Tetrahymena pyriformis, EC50, grw, 2 d, 13.7 mg/l (Schultz 1987).

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1607 • Phenyl salicylate 118-55-8

LC50 values to fishes, mg/l	1.09 1.25	96hr, Pimephales promelas 96hr, Ictalurus punctatus (Holcombe et al. 1984)
Other information about water organisms	LC50, > 3.44 mg/l, 96hr, snail (Holcombe et al. 1984)	

1608 • 1-Phenyl-3-pyrazolidone 92-43-2

NOEC values to algae, mg/l	10	rpd, schr, Selenastrum capricornutum (Verschueren 1983)
LC50 values to crustaceans, mg/l	10	act, Daphnia magna (Verschueren 1983)

1609 • Phenyl-xylylmethane 13540-50-6

Sumformula of the chemical	C15H16	
Water solubility, mg/l	< 100	(MITI 1992)
Boiling point, °C	295	(MITI 1992)
Log octanol/water coefficient, log Pow	5.65	(MITI 1992)
Total degradation in water	Biodegradation: 1% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	323–3340 498–2260	8w, Cyprinus carpio, conc 0.015 mg/l 8w, Cyprinus carpio, conc 0.0015 mg/l (MITI 1992)
LC50 values to fishes, mg/l	1.67	48hr, Oryzias latipes (MITI 1992)

1610 • Phenylacetate 122-79-2

Sumformula of the chemical	C8H8O2	
Log octanol/water coefficient, log Pow	1.49	(Sangster 1989)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 115 mg/l (Bringmann & Kühn 1980a).	
LOEC values to algae, mg/l	7.5 3	rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1980a) rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1976)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 3 mg/l protozoa (Entosiphon sulcatum): 10 mg/l (Bringmann & Kühn 1980a).	

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1611 • Phenylacetonitrile 140-29-4

Synonyms	α-Tolunitrile Benzeneacetonitrile Benzyl cyanide Benzyl nitrile (Cyanomethyl)benzene α-Cyanotoluene omega-Cyanotoluene 2-Phenylacetonitrile Phenylethanenitrile	
Sumformula of the chemical	C8H7N	
Molecular weight	117.14	
Specific gravity (water=1)	1.015	at 18 °C
Vapour density (air=1)	4.05	
Conversion factor, 1 ppm in air=	4.87	mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.21	ppm
Vapour pressure, mmHg	0.1	at 20 °C or at 30 °C
Water solubility, mg/l	100	(MITI 1992)
Melting point, °C	−23– -26 -23.8	 (MITI 1992)
Boiling point, °C	233.5	(MITI 1992)
Log octanol/water coefficient, log Pow	1.6 1.56	(Anon. 1986) (Sangster 1989)
Total degradation in water	Biodegradation: 77% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
Other information about degradation	Biodegradation by a mutant microorganism: 500 mg/l at 20 °C: parent: 84% disruption in 48hr mutant: 100% disruption in 12hr	
LD50 values to mammals in oral exposure, mg/kg	45.5 270	orl-mus orl-rat (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	10 2000 270	ipr-mus skn-rat skn-rbt (Sweet 1987)
LC50 values to mammals in inhalation exposure, mg/m^3	430	ihl-rat (Sweet 1987)
LDLo values to mammals in non-oral exposure, mg/kg	74.982 32 50	ipr-rat scu-mus scu-rbt (Sweet 1987)

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LCLo values to mammals in inhalation exposure, mg/kg	100	ihl-mus (Sweet 1987)
Other information about mammals	Skin and eye irritation data: skin, rabbit, 500 mg, 24hr, mild (Sweet 1987).	
Effects on amphibia	LDLo, 1100 mg/kg, subcutaneous, frog (Sweet 1987).	

1612 •Phenylacridinium thiocyanate 82679-88-7

Other information about mammals	LDfr = 25.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

1613 • 1-(N-Phenylamino)naphthalene 90-30-2

Sumformula of the chemical	C16H13N	
EINECS-number	2019830	
Water solubility, mg/l	60	20° C (MITI 1991)
Melting point, °C	62	(MITI 1992)
Boiling point, °C	335	528 mmHg (MITI 1992)
Log octanol/water coefficient, log Pow	4.28	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	427–2730 889–2490	8w, Cyprinus carpio, conc 0.1 mg/l 8w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be accumulated on a medium level (Anon. 1987).	
LC50 values to fishes, mg/l	7.9	48hr, Oryzias latipes (MITI 1992)

1614 • 4-Phenylazophenol 1689-82-3

LC50 values to fishes, mg/l	1.1	96hr, Pimephales promelas (Holcombe et al. 1984)

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1615 • Phenylcarbinol 100-51-6

Synonyms	Benzylalcohol α-Hydroxytoluene Phenylmethanol Benzenecarbitol Phenylmethyl alcohol α-Toluenol Benzenemethanol
Sumformula of the chemical	C7H8O

Use	Perfumes and flavours; solvent; intermediate; inks; surfactant; photographic developer for colour movie films; dyeing nylon filament, textiles and sheet plastics; solvent for dyestuffs, cellulose esters, casein, waxes, etc.; heat-sealing polyethylene films; intermediate for benzyl esters and ethers; bacteriostat; cosmetics, ointments, emulsions.
State and appearance	Colourless liquid.
Odour	Slight odour; sharp, burning taste. Mild aromatic.
Molecular weight	108.13 (
Specific gravity (water=1)	1.05 at 15/15 °C 1.040–1.050 at 25/25 °C
Vapour density (air=1)	3.72
Conversion factor, 1 ppm in air=	4.42 mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.226 ppm
Vapour pressure, mmHg	1 at 58 °C
Water solubility, mg/l	40000 at 17 °C 35000 at 20 °C 41000 (MITI 1992)
Melting point, °C	-15.19 (MITI 1992)
Boiling point, °C	205.45 (MITI 1992)
Flashing point, °C	105 100.5
Log octanol/water coefficient, log Pow	1.1 (Anon. 1986) 1.43 (Sax 1986) 2.83 (Sax 1986) 1.05 (Sangster 1989)
Adsorption/desorption	Absorption proportional to organic content of soil (Sax 1986).
Other physicochemical properties	Somewhat soluble in water; miscible with alcohol, ether, chloroform. Combustible. Autoign temperature 436 °C. Flammability: Slight fire hazard when exposed to heat or flame; can react with oxidizing materials.
Total degradation in water	Biodegradation: 92–96% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

Other information about degradation	Impact on biodegradation processes: inhibition of degradation of glucose by Pseudomonas fluorescens at: 350 mg/l; inhibition of degradation of glucose by Escherichia coli at: > 1000 mg/l (Bringmann & Kühn 1960). Biodegrades relatively quickly (Sax 1986). The degradation of 26 compound, including 23 alcohols showed that phenyl alcohols degrade only after the biodegradation of other organic matter. – A continuous flow laboratory aerator-mixer was used to study the biodegradation of synthetic organic compounds including benzyl alcohol by activated sludge. Actinomyces biodegraded monohydric alcohols. – The degradation of benzyl alcohol by 2 types of sludges was studied. One sludge came from a waste treatment plant and the other was a laboratory grown sludge. There was a marked difference in the number of organisms present in the sludge with the ability to degrade benzyl alcohol. The testing of the ability of the 2 sludges to oxidize benzyl alcohol was studied by Respirometry. From the oxygen uptake of the sludges, the percent of theoretical oxygen uptake was compared on the basis of equimolar substrate concentrations and theoretically complete oxidation. After 12hr the percent theoretical oxidation that occurred was 9% for the treatment plant activated sludge and 16% for the laboratory grown sludge. In a second experiment, the laboratory sludge was acclimated to benzyl alcohol. Benzyl alcohol was found to be metabolized by both benzyl alcohol and phenol acclimated laboratory sludge (Sax 1986).
Metabolism in microorganisms	Washed suspensions of Acinetobacter calcoaceticus NCIB 8250 metabolized benzyl alcohol via benzaldehyde, benzoate, and the 3-oxoadipate path. Benzyl alcohol dehydrogenase and benzaldehyde dehydrogenase II were repressed when A. calcoaceticus utilizes L-mandelate or phenyl glyoxylate. Benzyl alcohol metabolism was also suppressed during growth on benzoate. – An NAD-linked dehydrogenase has been isolated from a toluene cultured, gram negative, aerobic Pseudomonas which catalyzes the interconversion of benzyl alcohol and benzaldehyde. The enzyme is called benzyl alcohol dehydrogenase and is unstable with a half-life of a few hours under conventional conditions. – When microorganisms isolated from activated sludge were adapted to growth on an individual aromatic compound such as benzyl alcohol, they were capable of rapid growth at 100 mg/ml concentration. The adapted microorganism could utilize aromatic compounds as the sole source of energy. The micro-organisms tested include various bacteria, actinomycetes, and yeasts (Sax 1986).
Metabolism in plants	Major neutral metabolite in barley is benzyl-B-L-glucophyranoside (Sax 1986).

LD50 values to mammals in oral exposure, mg/kg	3100	orl-rat (Patty 1967)
	1230	orl-rat
	1580	orl-mus
	1040	orl-rbt
		(Sax 1986)
LD50 values to mammals in non-oral exposure, mg/kg	64	ivn-rat
	324	ivn-mus
	2000	skn-rbt
		(Sax 1986)
LC50 values to mammals in inhalation exposure, mg/m³	4420	ihl-rat, 8hr (Sax 1986)
LDLo values to mammals in non-oral exposure, mg/kg	400	ipr-rat
	1700	scu-rat
	50	ivn-dog
	9	par-dog
	10000	skn-cat
	60	ivn-cat
	400	ipr-gpg
		(Sax 1986)
LCLo values to mammals in inhalation exposure, ppm	1000	ihl-rat, 8hr (Sax 1986)

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Other information about mammals	Rat: inhalation: LC0: 200–300 ppm, 2hr Rat: inhalation: LC33: 200–300 ppm, 4hr Rat: inhalation: LC100: 200–300 ppm, 8hr (Patty 1967).
Health effects	Moderately toxic. Can cause headaches, vertigo, nausea, vomiting, and diarrhea (Sax 1986). Direct contact: skin and eyes; general sensation: slight hazard on ingestion. Skin irritation grade 4–capillary injection diluted. Eye irritation grade 8 – severe burns 0.5 ml 10% solution. Causes local irritation of skin and mucous membranes, headache, vertigo, nausea, vomiting and diarrhea. Faint aromatic odour; sharp burning taste (Sax 1986). May cause irritation if present in recreational waters (Sax 1986). Pure alcohol is irritating and corrosive. Aqueous concentrations up to 4% well tolerated. Produces transient anesthesia of mucous membranes. Ingestion of large volumes resuls in vomiting, diarrhea, CNS depression. Converted to benzoic and hippuric acids. One human fatality attributed to rectal administration of 45 ml. – Dermal application to humans of 0.1 g of 32% concentration in acetone was mildly irritating. – Exerts narcotic action. Low toxicity. High exposure can cause decrease in blood pressure, depressant effect on system and death through respiratory paralysis (Sax 1986). Skin and eye irritation: skn, rbt, 10 mg, 24hr, mild; eye, rbt, 0.750 mg, severe; skn, pig, 100%, moderate (Sax 1986).
LD50 values to birds in oral exposure, mg/kg	100 orl-Agelaius phoeniceus (Sax 1986) > 100 orl-Sturnus vulgaris (Schafer et al. 1983)
Effects on microorganisms	Bacteria: Escherichia coli: no effect at 1 g/l (McKee & Wolf 1971).
EC50 values to microorganism, mg/l	5082 Biodegradation inhibition (Vaishnav 1986)
LC50 values to fishes, mg/l	10 96hr, Lepomis macrochirus 15 96hr, Menidia beryllina (Dawson et al. 1977) 460 96hr, Pimephales promelas (Mattson et al. 1976) 770 48hr, Pimephales promelas 460 96hr, Pimephales promelas (Sax 1986)
Other information about water organisms	Algae: Scenedesmus: 96hr threshold effect at 24 °C: 640 ppm; Arthropoda: Daphnia: 48hr threshold toxic effect at 23 °C: 360 ppm (McKee & Wolf 1971). Escherichia coli, 96hr, 1000 mg/l, 27 °C, no effect (Sax 1986).
Other information	Air pollution high. May emit toxic vapours when heated (Sax 1986). Found in jasmine, hyacinth, ylang-ylang oils, and at least 24 other essential oils (Sax 1986).

1616 • Phenylethanoic acid 103-82-2

Sumformula of the chemical	C8H8O2	
pKa	4.31	(Sangster 1989)
Log octanol/water coefficient, log Pow	1.41	(Sangster 1989)

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1617 • 1-Phenylethanol 1517-69-7

Sumformula of the chemical	C8H10O
Log octanol/water coefficient, log Pow	1.42 (Sangster 1989)

1618 • 2-Phenylethanol 60-12-8

Synonyms	S-Phenylethylalcohol
Sumformula of the chemical	C8H10O
Boiling point, °C	204 (MITI 1992)
Log octanol/water coefficient, log Pow	1.36 (Sangster 1989)
Total degradation in water	Biodegradation: 87% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992). Ready biodegradability: Confirmed to be biodegradable (Anon. 1987).

1619 • 2-Phenylethyl amine 64-04-0

Synonyms	1-Amino-2-phenylethane
Sumformula of the chemical	C8H11N
Use	Organic synthesis, lab reagent, scintillation counter (CO2 absorber).
State and appearance	Liquid.
Odour	A fishy odour.
Specific gravity (water=1)	0.964
Water solubility, mg/l	> 100 (MITI 1992)
Boiling point, °C	197–198 (MITI 1992)
pKa	9.82 (Sangster 1989)
Log octanol/water coefficient, log Pow	1.41 (Anon. 1986) 1.41 (Sangster 1989)
Other physicochemical properties	Absorbs carbon dioxide from air, strong base. Soluble in water, alcohol and ether. Combustible.
Total degradation in water	Biodegradation: 58% by BOD (on the upward trend) period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

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1620 • Phenylglycidyl ether 122-60-1

Synonyms	1-Phenoxy-2,3-epoxypropane
Sumformula of the chemical	C9H10O2
State and appearance	Colourless liquid.
Specific gravity (water=1)	1.11
Water solubility, mg/l	> 1000 (MITI 1992)
Melting point, °C	3.5
Boiling point, °C	245
Chemical oxygen demand, g O2/g	2.18 5 days (Bridie et al. 1979)
Biochemical oxygen demand, g O2/g	0.14 5 days (Bridie et al. 1979)
Total degradation in water	Biodegradation: 33–63% by BOD (on the upward trend) period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).
LC50 values to fish, mg/l	43 96hr, Carassius auratus (Bridie et al. 1979)

1621 • Phenylmercuryacetate 62-38-4

Use	Slimicide used by the paper and pulp industry, fungicide.
Molecular weight	336.75
Vapour pressure, mmHg	0.000009 35 °C
Water solubility, mg/l	4370
Melting point, °C	149–153
Total degradation in soil	Quickly degraded by soil microorganisms (Verschueren 1983).
Total degradation in water	Quickly degraded by aquatic microorganisms (Verschueren 1983).
LD50 values to mammals in oral exposure, mg/kg	22 orl-rat (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	60 orl-ckn 71 orl-qal (Lewis & Sweet 1984)
LC50 values to fishes, mg/l	0.004 48hr, Salmo gairdneri 0.005 24hr, Salmo gairdneri (Kemp et al. 1973) 0.08 48hr, Cyprinus carpio 0.07 48hr, Carassius auratus (Hashimoto & Nishiuchi 1981) 0.037 96hr, Gambusia affinis 0.044 formulation 96hr, Gambusia affinis (Joshi & Rege 1980)

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1622 • 2-(Phenylmethyl)pyridine 101-82-6

Other information about water organisms	Tetrahymena pyriformis, EC50, grw, 2.5 d, 66.3 mg/l (Schultz et al. 1987).

1623 • 3-(Phenylmethyl)pyridine 620-95-1

Other information about water organisms	Tetrahymena pyriformis, EC50, grw, 2.5 d, 33.72 mg/l (Schultz et al. 1987).

1624 • p-Phenylphenol 92-69-3

Sumformula of the chemical	C12H10O	
EINECS-number	2021792	
Water solubility, mg/l	38	(MITI 1992)
Melting point, °C	164–167	(MITI 1992)
Log octanol/water coefficient, log Pow	3.52 3.2	(MITI 1992) (Anon. 1986)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).	
Bioconcentration factor, fishes	39–57 30–48	6w, Cyprinus carpio, conc 0.02 mg/l 6w, Cyprinus carpio, conc 0.002 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	4.27	48hr, Oryzias latipes (MITI 1992)

1625 • Phenylphosphinic acid 1779-48-2

Sumformula of the chemical	C6H7PO2	
Water solubility, mg/l	73000	(MITI 1992)
Melting point, °C	83–87	(MITI 1992)
Log octanol/water coefficient, log Pow	-0.56– -0.44 (MITI 1992)	
Bioconcentration factor, fishes	< 0.2–0.4 < 2.0–10	6w, Cyprinus carpio, conc 1 mg/l 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 1000	48hr, Oryzias latipes (MITI 1992)

1626 • 2-Phenylpyridine 1008-89-5

Sumformula of the chemical	C11H9N	
pKa	4.63	(Sangster 1989)

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Log octanol/water coefficient, log Pow	2.63	(Sangster 1989)
Other information about water organisms	Tetrahymena pyriformis, EC50, grw, 2.5 d, 76.17 mg/l (Schultz et al. 1987).	

1627 • 3-Phenylpyridine 1008-88-4

Other information about water organisms	Tetrahymena pyriformis, EC50, grw, 2.5 d, 48.54 mg/l (Schultz et al. 1987).

1628 • 4-Phenylpyridine 939-23-1

Sumformula of the chemical	C11H9N	
pKa	5.45	(Sangster 1989)
Log octanol/water coefficient, log Pow	2.59	(Sangster 1989)

1629 • Phenylurea 64-10-8

Sumformula of the chemical	C7H8N2O	
Log soil sorption coefficient, log Kom	1.11	(Sabljic 1987)

1630 • Phorate 298-02-2

Synonyms	0,0-Diethyl-S-(ethylthiomethyl)-phosphorodithioate	
Molecular weight	260.39	
Vapour pressure, mmHg	0.00084	20 °C
Water solubility, mg/l	50	
Boiling point, °C	118–120	
Log soil sorption coefficient, log Kom	2.58	(Sabljic 1987)
Half-life in soil, days	82	(Li et al. 1990)
LD50 values to mammals in oral exposure, mg/kg	1 20	orl-rat orl-gpg (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	2.5	skn-rat (Lewis & Sweet 1984)
LC50 values to mammals in inhalation exposure, mg/m³	11	1hr, ihl-rat (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	0.6 1 1 7.5 1.33	orl-dck orl-bwd (Lewis & Sweet 1984) orl-Agelaius phoeniceus orl-Sturnus vulgaris orl-Quiscalus quiscula (Schafer et al. 1983)

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LD50 values to birds in dermal exposure, mg/kg	203	skn-dck (Lewis & Sweet 1984)
LC50 values to crustaceans, mg/l	0.0001 0.0003 0.0006 0.009	96hr, Penaeus duorarum (Anon. 1981) (EPA 600/4-81-041) 96hr, Mysidopsis bahia (Anon. 1981) (EPA 600/4-81-041) 96hr, Gammarus fasciatus (Sanders 1972) 96hr, Gammarus lacustris (Sanders 1969)
LC50 values to fishes, mg/l	0.009 0.0013 0.0039 0.013 0.28	act, Salmo gairdneri (Kenaga 1979) 96hr, Cyprinodon variegetus (Anon. 1981) (EPA 600/4-81-041) 96hr, Leistomus canthurus (Anon. 1981) (EPA 600/4-81-041) 96hr, Salmo gairdneri (Pesticide Manual 1983) 96hr, Ictalurus punctatus (Pesticide Manual 1983)

1631 • Phorone 504-20-1

Synonyms	2,6-Dimethyl-2,5-heptadien-4-one	
Chemical oxygen demand, g O2/g	2.68	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g O2/g	0.19	5 days (Bridie et al. 1979)
LC50 values to fishes, mg/l	60	24hr, Carassius auratus (Bridie et al. 1979)

1632 • Phos-chek 7783-28-0

Synonyms	Phosphoric acid, diammonium salt	
Use	Fire prevention	
LC50 values to fishes, mg/l	224 105–230 94–165	XA, 96hr, Salmo gairdneri (Blahm 1979) 202, 96hr, Salmo gairdneri (Johnson & Sanders 1977) 259, 96hr, Salmo gairdneri (Johnson & Sanders 1977)

1633 • Phosfolan 947-02-4

Synonyms	Phospholan	
Other information about mammals	ALD = 42 mg/kg, act, orl, deer mouse LDfr = 87.5 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).	
LD50 values to birds in oral exposure, mg/kg	2.37 5.62 23.7 2.37 2.37 2.37 1.78	orl-Agelaius phoeniceus orl-Sturnus vulgaris orl-Coturnix coturnix orl-Passer domesticus orl-Quiscalus cuiscula orl-Columba livia orl-Quelea quelea (Schafer et al. 1983)

1634 • Phosphoric acid 7664-38-2

Synonyms	Orthophosphoric acid
Sumformula of the chemical	H3O4P

Use	Active ingredient in herbicides.
Molecular weight	98
LD50 values to mammals in oral exposure, mg/kg	1530 orl-rat (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	2740 skn-rbt (Sweet 1987)
Other information about mammals	Skin and eye irritation: skin, rabbit, 595 mg, 24hr, severe; eye, rabbit, 119 mg, severe (Sweet 1987).

1635 • Phosphoric acid, trisodium salt 7601-54-9

Synonyms	Sodium phosphate Sodium phosphate, anhydrous Sodium phosphate, tribasic Trisodium orthophosphate Trisodium phosphate
Sumformula of the chemical	O4P.3Na
Molecular weight	163.94
LDLo values to mammals in non-oral exposure, mg/kg	1580 ivn-rbt (Sweet 1987)
Mutagenicity	Mutation data: sin, orl, 11 pph (Sweet 1987).

1636 • Photoaldrin 13350-71-5

LC50 values to fishes, mg/l	0.009 24hr, Lepomis macrochirus (Khan et al. 1973)
Other information about water organisms	LC50 (24hr), 0.0005 mg/l, Aedes aegypti (Khan et al. 1973).
Other information	When aldrin photolyses → photoaldrin.

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1637 • Photoheptachlor 33442-83-0

LC50 values to fishes, mg/l	0.008 24hr, Pimephales promelas (Khan et al. 1973)
Other information about water organisms	LC50 (24hr), 0.002 mg/l, Aedes aegypti (Khan et al. 1973).
Other information	When heptachlor photolyses → photoheptachlor.

1638 • Photoisodrin 3212-28-0

LC50 values to fishes, mg/l	0.025 24hr, Lepomis macrochirus 0.01 24hr, Pimephales promelas (Khan et al. 1973)
Other information	When isodrin photolyses → photoisodrin

1639 • Phoxim

14816-18-3

Synonyms	0,0-Diethyl-0-(α-cyanobenzylideneamino)thiophosphate
Use	Active ingredient in insecticides.
Water solubility, mg/l	< 10 (MITI 1992)
Log octanol/water coefficient, log Pow	4.38 (MITI 1992)
Total degradation in water	Biodegradation: 3–8% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	781–1610 8w, Cyprinus carpio, conc 0.0166 mg/l 412–1020 8w, Cyprinus carpio, conc 0.00166 mg/l (MITI 1992)
LD50 values to birds in oral exposure, mg/kg	10 orl-Agelaius phoeniceus 23.7 orl-Sturnus vulgaris 23.7 orl-Coturnix coturnix 5.62 orl-Passer domesticus 75 orl-Quiscalus quiscula 23.7 orl-Columba livia (Schafer et al. 1983)
LC50 values to fishes, mg/l	0.1–1.0 act, Salmo gairdneri (Pesticide Manual 1983) 0.1–1.0 act, Cyprinus carpio (Pesticide Manual 1983) 1–10 act, Carassius auratus (Pesticide Manual 1983) 3.16 48hr, Oryzias latipes (MITI 1992)

1640 • Phthalazine

253-52-1

EC50 values to algae, mg/l	18	5d, Selenastrum capricornutum (Lande et al. 1987)
EC50 values to crustaceans, mg/l	445	2d, Daphnia magna (Lande et al. 1987)
LC50 values to fishes, mg/l	100	4d, Pimephales promelas (Lande et al. 1987)

1641 • Phthalic acid anhydride

85-44-9

Synonyms	Phthalic anhydride 1,2-Benzenedicarboxylic acid anhydride 1,3-Dioxophthalan 1,3-Isobenzofurandione 1,3-Pthalandione
Sumformula of the chemical	C8H4O3
Use	Alkyd resins, plasticizers, hardener for resins, polyesters, synthesis of phenolphthalein and phthaleins, many other dyes, chlorinated products, pharmaceutical intermediates, insecticides, diethyl phthalate, dimethyl phthalate, laboratory reagent.
State and appearance	White crystalline needles.
Odour	Mild odour.
Molecular weight	148.12

PQR

Vapour density (air=1)	5.1
Vapour pressure, mmHg	1 96.5 °C 0.0002 at 20 °C (Verschueren 1983)
Water solubility, mg/l	6200 at 25 °C (Towle et al. 1968)
Melting point, °C	131–132 (MITI 1992)
Boiling point, °C	284.5 (MITI 1992)
Sublimation point, °C	295
Flashing point, °C	151.6
Henry's law constant, Pa x m³/mol	0.00063 calc. (Lyman et al. 1982)
Adsorption/desorption	A Koc of 36 has been estimated. Based on this estimated Koc, phthalic anhydride will not adsorb to soils or sediments (Kenaga 1980). Corrosive. Combustible when exposed to heat or flame; can react with oxidizing materials. Moderate explosion hazard in the form of dust when exposed to flame. The production of this material has caused many industrial explosions. Mixtures with copper oxide or sodium nitrite explode when heated. Violent reaction with nitric acid + sulfuric acid above 80 °C (Sax & Lewis 1989). Soluble in alcohol, carbon disulfide, and hot water.
Photochemical degradation in air	Phthalic anhydride adsorbs light > 290 nm and may therefore be susceptible to direct sunlight photo lysis. The estimated vapour phase half-life in the atmosphere is 1.00 days, as a result of addition of photochemically produced hyrdoxyl radicals (Sadtler 1966) (GEMS 1986).
Other reactions in atmosphere	A common air contaminant (Sax & Lewis 1989).
Hydrolysis in water	Phthalic anhydride hydrolyses rapidly in water. An estimated half-life of approx 1.5 min was calculated using a observed rate constant of 7.9 x 10-3 sec-1 for hydrolysis in aqueous solution at 25 °C (Towle et al. 1968) (Hawkins 1975).
Total degradation in water	Biodegradation: 85.2% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
Other information about degradation	Percent theoretical BOD was reported to be 44–78 as a result of incubation of 1–4 ppm with sewage inoculum (Heukelekian & Rand 1955). Degradation of an initial concentration of 2 ppm phthalic anhydride was approx 21% after incubation with sewage (standard dilution method) and 18% (seawater dilution method) for 5 days (Takemoto et al. 1981). Mineralization of 33% of an initial concn of 9 ppm phthalic anhydride incubated with activated sludge for 24hr was reported based on COD (Matsui et al. 1975). Phthalic anhydride was reported to be significantly degraded in Japanese MITI tests using activated sludge as inoculum (Sasaki 1978). Percent theoretical BOD was 73.46% in 5 days using dilution water seeded with domestic sewage (Swope & Kenna 1950).
Bioconcentration factor, algae	4053 Oedogonium (Lu & Metcalf 1975)
Other information about bioaccumulation	Phthalic anhydride did not bioconcentrate in Daphnia, Physa (snail) or Gambusia (fish) (Ly & Metcalf 1975).
LD50 values to mammals in oral exposure, mg/kg	4020 orl-rat 2000 orl-mus (Sax & Lewis 1989)

LDLo values to mammals in oral exposure, mg/kg	100	orl-gpg (Sax & Lewis 1989)
TDLo values to mammals in non-oral exposure, mg/kg	203	ipr-mus, 8-10d preg, teratogenic (Sax & Lewis 1989)
Health effects	skn, rbt, 500 mg, 24hr, mild; eye, rbt, 100 mg, severe (Sax & Lewis 1989). Poison by ingestion. Experimental teratogenic effects. A corrosive eye, skin and mucous membrane irritant (Sax & Lewis 1989).	
Carcinogenicity	NCI carcinogenesis bioassay (feed); No evidence: mouse, rat (Sax & Lewis 1989).	

1642 • o-Phthalonitrile 91-15-6

Sumformula of the chemical	C8H4N2	
EINECS-number	2020448	
Water solubility, mg/l	395	(MITI 1992)
Melting point, °C	141	(MITI 1992)
Log octanol/water coefficient, log Pow	0.74	(MITI 1992)
Total degradation in water	Biodegradation: 3.3% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	8.8–1.3 < 5.5	6w, Cyprinus carpio, conc 0.2 mg/l 6w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	29	48hr, Oryzias latipes (MITI 1992)

1643 • Physostigminesulfate 64-47-1

Other information about mammals	ALD = 10.0 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987).

1644 • Picloram 1918-02-1

Synonyms	4-Amino-3,5,6-trichloropicolinic acid	
Use	Herbicide.	
Molecular weight	241.46	
Vapour pressure, mmHg	0.000000616, 35 °C	
Water solubility, mg/l	430	25 °C
Log soil sorption coefficient, log Kom	1.23	(Sabljic 1987)
Half-life in soil, days	100	(Li et al. 1990)
Total degradation in soil	75–100% disappearance from soils: 18 months (Verschueren 1983).	

LD50 values to mammals in oral exposure, mg/kg	2898 orl-rat 1061 orl-mus (Lewis & Sweet 1984)
Carcinogenicity	NCI carcinogenesis bioassay completed: results positive: rat; results negative, mus (Lewis & Sweet 1984).
LD50 values to birds in oral exposure, mg/kg	4000 orl-ckn (Lewis & Sweet 1984)
Effects on plants	In greenhouse trials, seedling emergence and dry weight production of both creeping red fescue (Festuca rubra) and timothy (Pleum pratense) were partly or completely inhibited by preplant treatment of the pots with picloram at 0.28 kg/ha or more (Gallagher & Vanden Born 1976).
EC50 values to algae, mg/l	100 rpd, 10 d, Chlorococcum sp. Phaeodactylum tricornutum 50 rpd, 10d, Isochrysis galbana (Walsh 1972)
LC50 values to crustaceans, mg/l	34.4 act, Daphnia magna (Kenaga 1979) 27 96hr, Gammarus lacustris (Sanders 1969) 68.3 48hr, Daphnia magna (Gersich et al.1985) 50.7 48hr, Daphnia magna (Mayes & Dill 1984)
LC50 values to fishes, mg/l	21.9 96hr, Lepomis macrochirus 44.5 96hr, Lepomis macrochirus 55.3 96hr, Pimephales promelas 19.3 96hr, Salmo gairdneri (Mayes & Dill 1984) 1.55–4.95 96hr, Salmo trutta m. lacustris (Woodward 1976) 4.3 96hr, Salvelinus namaycush 12.5 96hr, Salmo gairdneri 4.8 96hr, Salmo clarci 23 96hr, Lepomis macrochirus 6.3–15.5 96hr, Ictalurus punctatus (Johnson & Finley 1980) 4.5 96hr, Salmo clarci (Woodward 1982) 120 96hr, Gambusia affinis (Johnson 1978) 5.5 96hr, Salmo gairdneri 14.5–44.5 96hr, Lepomis macrochirus (Mayes & Oliver 1985) 26 96hr, Jordanella floridae 36 96hr, Branchydanio rerio 26 96hr, Salmo gairdneri (Fogels & Sprague 1977) 21 act, Lepomis macrochirus 24 act, Salmo gairdneri (Kenaga 1979) 20 24hr, Oncorhynchus kisutch 17.5 24hr, Oncorhynchus kisutch (Lorz et al. 1979) 15.6 4d, Salmo gairdneri 14 8d, Salmo gairdneri (Mayes et al. 1987)
LOEC values to fishes, mg/l	0.035 srv, grw, Salmo trutta m. lacustris (Woodward 1976)
Effects on the physiology of water organisms	Salmo gairdneri, 0.550 mg/l, 70 d, measurable change in length and/or weight (Mayes et al. 1987).

1645 • Picric acid 88-89-1

Synonyms	Carbazotic acid 2-Hydroxy-1,3,5-trinitrobenzene Nitroxanthic acid 2,4,6-Trinitrophenol Phenol trinitrate Picronitric acid 1,3,5-Trinitrophenol
Sumformula of the chemical	C6H3N3O7
Molecular weight	229.12
Bioconcentration factor, fishes	< 0.24 6w, Cyprinus carpio, conc 0.5 mg/l < 2.2 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LDLo values to mammals in oral exposure, mg/kg	250 orl-cat 120 orl-rbt 100 orl-gpg (Lewis & Sweet 1984)
LDLo values to mammals in non-oral exposure, mg/kg	60 scu-dog 60 unk-dog (Lewis & Sweet 1984)
Effects on amphibia	LDLo, 200 mg/kg, scu-frg (Lewis & Sweet 1984).
LC50 values to crustaceans, mg/l	85 48hr, Daphnia magna (LeBlanc 1984)
LC50 values to fishes, mg/l	230 48hr, Oryzias latipes (MITI 1992)
Other information about water organisms	LC (48hr) 117 mg/l, Oryzias latipes (Tonogai et al. 1982). LC (48hr) 170 mg/l, Lepomis macrochirus (Buccafusco et al. 1981).

1646 • Pigment Blue-15 147-14-8

Synonyms	Copper, (29H,31H-phthalocyaninato(2-)-N 29, N 30, N 31, N 32)- (SP-4-1)-
Sumformula of the chemical	C32H16CuN8
EINECS-number	2056851
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.33–11 6w, Cyprinus carpio, conc 0.6 mg/l < 3.6 6w, Cyprinus carpio, conc 0.06 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	> 100 48hr, Oryzias latipes (MITI 1992)

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1647 • Pigment Green-7 1328-53-6

Water solubility, mg/l	< 1 (MITI 1992)
Bioconcentration factor, fishes	0.51–4.8 6w, Cyprinus carpio, conc 0.1 mg/l < 2.1–74 6w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	> 250 48hr, Oryzias latipes (MITI 1992)

1648 • Pigment Orange-13 3520-72-7

Sumformula of the chemical	C32H24C12N8O2
Melting point, °C	330 (MITI 1992)
Bioconcentration factor, fishes	0.75–5.6 6w, Cyprinus carpio, conc 0.15 < 2.8 6w, Cyprinus carpio, conc 0.015 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	> 100 48hr, Oryzias latipes (MITI 1992)

1649 • Pigment Red-53 5160-02-1

Sumformula of the chemical	C17H12ClN2O4S.1/2Ba
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	0.9–1.8 6w, Cyprinus carpio, conc 0.7 mg/l 8.5–15 6w, Cyprinus carpio, conc 0.07 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	> 420 48hr, Oryzias latipes (MITI 1992)

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1650 • Pigment Red-57-9 5281-04-9

Water solubility, mg/l	< 100 (MITI 1992)
Melting point, °C	> 300 (MITI 1992)
Total degradation in water	Biodegradation: 9–12% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

Bioconcentration factor, fishes	< 0.7–1.8 < 6.9	6w, Cyprinus carpio, conc 0.3 mg/l 6w, Cyprinus carpio, conc 0.03 mg/l (MITI 1992)
LC50 values to fishes, mg/l	50	48hr, Oryzias latipes (MITI 1992)

1651 • Pigment Yellow-12

6358-85-6

Sumformula of the chemical	C32H26C12N6O4	
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	0.38–3.2 2.4–5.4	6w, Cyprinus carpio, conc 0.1 mg/l 6w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	> 420	48hr, Oryzias latipes (MITI 1992)

1652 • Pilocarpine-HCl

54-71-7

Other information about mammals	ALD = 80.0 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987).

1653 • Pimaric acid

510-39-4

Synonyms	Levopimaric acid	
Use	Resins.	
LC50 values to fishes, mg/l	0.33	96hr, Salmo gairdneri (Anon. 1981)
	0.32	96hr, Oncorhynchus kisutch (Leach & Thakore 1978)
	0.37	96hr, Oncorhynchus kisutch (Rogers 1975)
	0.8	96hr, Salmo gairdneri (Leach & Thakore 1976)

1654 • 2-Pinene

80-56-8

LC50 values to crustaceans, mg/l	41	48hr, Daphnia magna (LeBlanc 1980)

1655 • Piperazine

110-85-0

Melting point, °C	42	(MITI 1992)
Boiling point, °C	125–130	(MITI 1992)

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Total degradation in water	Biodegradation: 1.4% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	0.3–0.9 6w, Cyprinus carpio, conc 1 mg/l < 3.9 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	> 1000 48hr, Oryzias latipes (MITI 1992)

1656 • Piperidine 110-89-4

Sumformula of the chemical	C5H11N
EINECS-number	2038130
Melting point, °C	-13 (MITI 1992)
Boiling point, °C	106 (MITI 1992)
Total degradation in water	Biodegradation: 66.9% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

1657 • Piperonal 120-57-0

Synonyms	1,3-Benzodioxole-5-carboxaldehyde
Sumformula of the chemical	C8H6O3
EINECS-number	2044097
Water solubility, mg/l	2000 (MITI 1992)
Melting point, °C	37 (MITI 1992)
Boiling point, °C	263 (MITI 1992)
Total degradation in water	Biodegradation: 88.0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

1658 • Pirimicarb 23103-98-2

Synonyms	2-Dimethylamino-5,6-dimethylpyrimidine-4-yl-dimethylcarbamate
Use	Active ingredient in insecticides.
LC50 values to fishes, mg/l	55 96hr, Lepomis macrochirus 29 96hr, Salmo gairdneri (Pesticide Manual 1983)

1659 • Piror P 72 * 73482-03-8

Active ingredients	2-Bromo-2-nitropropane-1,3-diol * 18%; 2-Hydroxymethyl-2-nitropropane-1,3-diol * 3.5%	
Use	Pesticide; slimicide.	
LC50 values to crustaceans, mg/l	10	96hr, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	39	96hr, Alburnus alburnus (Linden et al. 1979)

1660 • Pivalic acid 75-98-9

Synonyms	2,2-Dimethylpropionic acid 2,2-Dimethylpropanoic acid	
Water solubility, mg/l	22000	(MITI 1992)
Melting point, °C	35.3–35.5	(MITI 1992)
Boiling point, °C	163.7–163.8	(MITI 1992)
Log octanol/water coefficient, log Pow	1.48	(MITI 1992)
Chemical oxygen demand, g 02/g	1.94	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.21	5 days (Bridie et al. 1979)
Bioconcentration factor, fishes	< 0.2–1.2 < 2.3	6w, Cyprinus carpio, conc 1 mg/l 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
LC50 values to fishes, mg/l	375 4500 217	96hr, Carassius auratus (Anon. 1975) 24hr, Carassius auratus (Bridie et al. 1979) 48hr, Oryzias latipes (MITI 1992)

1661 • Platinium and platinium compounds 7440-06-4

Molecular weight	195.09	
Effects on plants	Horticultural crops were exposed to 0.057, 0.57 and 5.7 ppm Pt in Hoaglands solution for a week. Chlorosis of young tissue (roots and shoots) was usually evidenced and dry weights of 5 species were significantly reduced by 5.7 ppm (Pallas & Jones 1978).	
LC50 values to crustaceans, mg/l	0.52	21d, Daphnia magna (Biesinger & Christensen 1972)
EC50 values to crustaceans, mg/l	0.082	21d, rpd, Daphnia magna (Biesinger & Christensen 1972)
LOEC values to crustaceans, mg/l	0.014	21d, rpd, Daphnia magna (Biesinger & Christensen 1972)
LC50 values to fishes, mg/l	5.2 2.5	48hr, Oncorhynchus kisutch 96hr, Oncorhynchus kisutch (Ferreira & Wolke 1979)

PQR

1662 • Poly(1,3-butanediol, adipic acid)ester 60108-89-6

Total degradation in water	Biodegradation: 87% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

1663 • Poly(degree of polymerization=10) oxyethylene p-nonylphenyl ether 26027-38-3

Sumformula of the chemical	(C2H4O)nC15H24O
Water solubility, mg/l	> 1000 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 21d substance: 30 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	9.09–16.0 6w, Cyprinus carpio, conc 1 mg/l 7.6–12.4 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	11.6 48hr, Oryzias latipes (MITI 1992)

1664 • Poly(methylene ether) 9002-81-7

Sumformula of the chemical	CnH4On
Melting point, °C	110–140 (MITI 1992)
Total degradation in water	Biodegradation: 87–96% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

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1665 • Polychlorinated triphenyls 12642-23-8

Synonyms	PCT
Sumformula of the chemical	C18H9Cl5 * Aroclor 5442
Products containing the chemical	Aroclor 5442 Aroclor 5460 * 60% chlorine
Use	Aroclor 5442 is used in heat transfer, hydraulic fluids, lubricants and insecticides.
Molecular weight	400; 575

Log octanol/water coefficient, log Pow	5.5	Aroclor 5442 (Anon. 1989)
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).	
Other information about degradation	Less persistent against photo- and biodegradation than PCB (Fawell & Hunt 1988).	
Metabolism in mammals	Mouse and rat: strong accumulation in liver and in kidney, heart and fat tissue, induction of the microsom cytocrom P-450 system in liver (Fawell & Hunt 1988).	
Other information about bioaccumulation	Confirmed to be accumulated on a medium level (Anon. 1987). Little laboratory data available, but occurrence in oysters, fish and fish eating animals indicate bioaccumulation and biomagnification in food chain (Addison et al. 1972). Direct uptake and bioaccumulation in cod have been indicated (Addison et al. 1972).	
LD50 values to mammals in oral exposure, mg/kg	10600	orl-rat, Aroclor 5442 (Sax & Lewis 1989)
LD50 values to mammals in non-oral exposure, mg/kg	3160	skn-rbt, Aroclor 5442 (Sax & Lewis 1989)
Effects on the physiology of mammals	Rhesus ape: 5000 mg/kg in food, 3 months, decreased weight, hair fall down, oedema, changes in liver, injuries in the mucous membrane of the stomach (Allen & Norback 1973).	
Health effects	Moderately toxic by skin contact. Mildly toxic by ingestion. When heated to decomposition it emits toxic fumes of Cl- (Sax & Lewis 1989).	
Carcinogenicity	Mouse, 24 weeks study induced liver tumors (Shirai et al. 1978).	
Effects on the reproduction of birds	Chicken, 20 mg/kg with food, increased amount of deaths and abnormal embryos (Cecil et al. 1974).	
LC50 values to fishes, mg/l	> 50	96hr, Salmo clarki (Mayer & Ellersieck 1986)

1666 • Polychlorobiphenyl (Cl = 2) 25512-42-9

Sumformula of the chemical	C12H8Cl2	
Total degradation in water	Biodegradation: 12.8% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	1120–10300 600–16000	8w, Cyprinus carpio, conc 0.0066 mg/l 8w, Cyprinus carpio, conc 0.0022 mg/l (MITI 1992)
LC50 values to fishes, mg/l	2.2	48hr, Oryzias latipes (MITI 1992)

1667 • Polychlorobiphenyl (Cl = 3) 25323-68-6

Sumformula of the chemical	C12H7Cl3
Total degradation in water	Biodegradation: 2% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

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Bioconcentration factor, fishes	5900–20200 5500–15900	4w, Cyprinus carpio, conc 0.0054 mg/l 4w, Cyprinus carpio, conc 0.0018 mg/l (MITI 1992)
LC50 values to fishes, mg/l	1.8	48hr, Oryzias latipes (MITI 1992)

1668 • Polychlorobiphenyl (Cl = 4) 26914-33-0

Sumformula of the chemical	C12H8Cl4	
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	8100–21900 5100–19800	4w, Cyprinus carpio, conc 0.0063 mg/l 4w, Cyprinus carpio, conc 0.0021 mg/l (MITI 1992)
LC50 values to fishes, mg/l	2.1	48hr, Oryzias latipes (MITI 1992)

1669 • Polychlorobiphenyl (Cl = 6) 26601-64-9

Sumformula of the chemical	C12H8Cl6	
Total degradation in water	Biodegradation: 0.8% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	1700–7700 2500–9400	4w, Cyprinus carpio, conc 0.042 mg/l 4w, Cyprinus carpio, conc 0.014 mg/l (MITI 1992)
LC50 values to fishes, mg/l	14	48hr, Oryzias latipes (MITI 1992)

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1670 • Polychloronaphthalene (Cl = 3-5) 38289-27-9

Sumformula of the chemical	C10H7Cl3-5	
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).	
Bioconcentration factor, fishes	5600–11800 4400–8500	8w, Cyprinus carpio, conc 0.05 mg/l 8w, Cyprinus carpio, conc 0.005 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be accumulated on a high level (Anon. 1987).	
LC50 values to fishes, mg/l	7.2	48hr, Oryzias latipes (MITI 1992)

1671 • Polydimethylsiloxane 9016-00-6

LC50 values to fishes, mg/l	> 10000 96hr, Salmo gairdneri (Hobbs et al. 1975)

1672 • Polyethylene glycol 25322-68-3

Synonyms	Polyoxyethylene
Total degradation in water	Biodegradation: n=4 56.2% by BOD (on the upward trend) n=10 53.0% by BOD (on the upward trend) period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
LC50 values to fishes, mg/l	> 5000 24hr, Carassius auratus (Anon. 1975)

1673 • Polyethylene glycol monomethyl ether (n = 4 or 5) 23783-42-8 (n=4) 23778-52-1 (n=5)

Sumformula of the chemical	C9(11)H20(24)O5(6)
Water solubility, mg/l	< 100000 (MITI 1992)
Melting point, °C	< -10 (MITI 1992)
Boiling point, °C	295 (MITI 1992)
Total degradation in water	Biodegradation: 24–85% by BOD (on the upward trend) period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).

1674 • Polyoxyethylene dodecyl ether 9002-92-0

Sumformula of the chemical	(C2H4)n.C12H26O
Water solubility, mg/l	> 10000 (MITI 1992)
Total degradation in water	Biodegradation: 74% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

1675 • Polypropylene glycol 25322-69-4

LC50 values to fishes, mg/l	1700 96hr, Lepomis macrochirus 650 96hr, Menidia audens (Dawson et al. 1977)

PQR

1676 • Polyram 9006-42-2

Use	Fungicide.	
LC50 values to fish, mg/l	17	48hr, Rasbora heteromorpha (Martin 1968)

1677 • Polystyrene (average molecular weight ca. 800) 9003-53-6

Sumformula of the chemical	(C8-H8)x	
Water solubility, mg/l	< 10	(MITI 1992)
Boiling point, °C	> 300	(MITI 1992)
Total degradation in water	Biodegradation: 1–3% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	58–144 358–821	8w, Cyprinus carpio, conc 2 mg/l 8w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 500	48hr, Oryzias latipes (MITI 1992)

1678 • Polyvinyl alcohol 9002-89-5

Sumformula of the chemical	(C2H4O)x	
Bioconcentration factor, fishes	< 0.99 < 7.5	6w, Cyprinus carpio, conc 4 mg/l 6w, Cyprinus carpio, conc 0.4 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	> 1000	48hr, Oryzias latipes (MITI 1992)

PQR

1679 • Potassium and potassium compounds 7440-09-7

LC50 values to crustaceans, mg/l	97 93 166 450	21d, Daphnia magna 48hr, without food, D.magna 48hr, with food, D.magna (Biesinger & Christensen 1972) 96hr, Nitocra spinipes (Bengtsson 1978)
EC50 values to crustaceans, mg/l	68	rpd, 21 d, Daphnia magna (Biesinger & Christensen 1972)
LOEC values to crustaceans, mg/l	53	rpd, 21 d, Daphnia magna (Biesinger & Christensen 1972)

1680 • Potassium carbonate 584-08-7

Synonyms	Carbonic acid, dipotassium salt Potash

Sumformula of the chemical	CO3.2K	
Molecular weight	138.21	
LD50 values to mammals in oral exposure, mg/kg	1870	orl-rat (Sweet 1987)
LD50 values to birds in oral exposure, mg/kg	100 100	orl-bdw (Sweet 1987) orl-Agelaius phoeniceus (Schafer et al. 1983)

1681 • Potassium chloride

7447-40-7

Synonyms	Dipotassium dichloride Potassium monochloride Tripotassium trichloride	
Sumformula of the chemical	ClK	
Molecular weight	74.55	
LD50 values to mammals in oral exposure, mg/kg	2500 383 2600	orl-gpg orl-mus orl-rat (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	1181 660 117 39	ipr-mus ipr-rat ivn-mus ivn-rat (Sweet 1987)
LDLo values to mammals in oral exposure, mg/kg	938 20	orl-infant orl-man (Sweet 1987)
LDLo values to mammals in non-oral exposure, mg/kg	85 900 2550	ipr-dog ipr-gpg scu-gpg (Sweet 1987)
TDLo values to mammals in oral exposure, mg/kg	60	orl-wmn, gastrointestinal, blood,1d (Sweet 1987)
Other information about mammals	Skin and eye irritation data: eye, rabbit, 500 mg, 24hr, mild (Sweet 1987).	
Mutagenicity	Mutation data: cyt, ham, lug, 12000 mg/l; mrc, smc, 400 mmol/l; microbial mutation without S9, sat, 0.1 mg/plate; microbial mutation without S9, smc, 2500 mmol/l; mma, sat, 0.1 mg/plate; sin, smc, 300 mmol/l (Sweet 1987).	
Other information about birds	LDLo, scu, 2210 mg/kg, pigeon (Sweet 1987).	
Effects on amphibia	LDLo, scu, frog, 2120 mg/kg (Sweet 1987).	
LC50 values to fishes, mg/l	2010	96hr, Lepomis macrochirus (Kemp et al. 1973)

PQR

1682 • Potassium chromate 7789-00-6

Sumformula of the chemical	K2Cr04
Water solubility, mg/l	629000 20 °C
EC50 values to crustaceans, mg/l	2.69 2d, mbt, Crangonyx pseudogracilis 0.81 4d, mbt, Crangonyx pseudogracilis (Martin & Holdich 1986) 0.024–0.170 2d, Daphnia pulex (Dorn et al. 1987)

1683 • Potassium chromic sulfate 10141-00-1

LC50 values to fishes, mg/l	750 96hr, Salmo gairdneri (Sprague & Logan 1979)

1684 • Potassium cyanide 151-50-8

Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 0.001 mg/l (Bringmann & Kühn 1980a).
Effects on the physiology of water organisms	Salmo gairdneri, 0.009 mg/l, 1 d, change in enzyme activity (Raymond et al. 1986).
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 0.03 mg/l protozoa (Entosiphon sulcatum): 1.8 mg/l (Bringmann & Kühn 1980a).

1685 • Potassium dichromate 7778-50-9

Molecular weight	294.2
LDLo values to mammals in oral exposure, mg/kg	26 orl-chd (Lewis & Sweet 1984)
Effects on amphibia	NOEC, 1 mg/l, 100d, Xenopus laevis, mortality. NOEC, 3.2 mg/l, 100d, Xenopus laevis, development. NOEC, 3.2 mg/l, 100d, Xenopus laevis, growth. (Slooff & Canton 1983)
Effects on arthropods	NOEC, 3.2 mg/l, 25d, Culex pipiens, mortality. NOEC, 3.2 mg/l, 25d, Culex pipiens, development. (Slooff & Canton 1983)
Effects on plants	NOEC, 0.32 mg/l, 7d, Lemna minor, Specific growth rate. (Slooff & Canton 1983)
Effects on microorganisms	NOEC, 0.32 mg/l, 0.3d, Pseudomonas fluorescens, specific growth rate. NOEC, 1 mg/l, 0.3d, Microcystis aeruginosa, specific growth rate. (Slooff & Canton 1983)
NOEC values to algae, mg/l	0.32 rpd, schr, 96hr, Scenedesmus pannonicus (Slooff & Canton 1983)
LC50 values to crustaceans, mg/l	0.1–0.2 24hr, Daphnia magna (SFS 5062) 1.1 48hr, Daphnia magna (Hermens et al. 1984) 16 96hr, Nitocra spinipes (Linden et al. 1979) 2.4 1d, Daphnia magna 1.8 2d, Daphnia magna (Khangarot et al. 1987) 0.5 21d, Daphnia magna van Leeuwen et al. 1987

PQR

EC50 values to crustaceans, mg/l	0.27 rpd, schr, 16 d, Daphnia magna (Hermens et al. 1984) 0.03 2d, Ceriodaphnia sp. (Dorn et al. 1987) 2.2 2d, mbt, Crangonyx pseudogracilis 0.42 4d, mbt, Crangonyx pseudogracilis (Martin & Holdich 1986) 0.64 Daphnia magna (van Leeuwen et al. 1987) 2.2 1d, mbt, Daphnia magna 1.79 2d, mbt, Daphnia magna (Khangarot & Ray 1987) 0.020–0.170 2d, Daphnia pulex (Dorn et al. 1987)
NOEC values to crustaceans, mg/l	0.1 srv, chr, 21 d, Daphnia magna (Slooff & Canton 1983)
LC50 values to fishes, mg/l	113 96hr, Lepomis macrochirus (Kemp et al. 1973) 240 96hr, Alburnus alburnus (Linden et al. 1979) 26.13 4d, Pimephales promelas 148.31–201.24 4d, Lepomis macrochirus (Dorn et al. 1987)
NOEC values to fishes, mg/l	10 srv, 28d, Poecilia reticulata 10 srv + bhv, 28d, Poecilia reticulata 10 grw, 28d, Poecilia reticulata 10 srv, 40d, Oryzias latipes 10 srv + bhv, 40d, Oryzias latipes 100 grw, 40d, Oryzias latipes (Slooff & Canton 1983)
Effects on the physiology of water organisms	Anacystis nidulans; Spirulina platensis: 0.010 mg/l, 0.25 d, photosynthesis effect (change in plant productivity) (Azeez & Banerjee 1987). Branchydanio rerio, > 85.0 mg/l, 16 d, change in percent hatch or time to hatch (Dave et al. 1987).
Other information about water organisms	NOEC, 3.2 mg/l, 21d, Hydra oligactis, specific growth rate. NOEC, 10 mg/l, 21d, Lymnaea stagnalis, mortality. NOEC, 0.32 mg/l, 21d, Lymnaea stagnalis, reproduction. NOEC, 1 mg/l, 21d, Lymnaea stagnalis, hatching. (Slooff & Canton 1983)
Other information	Toxicity decreases when the hardness of water increases (Bergling & Dave 1984).

1686 • Potassium hydroxide 1310-58-3

Synonyms	Caustic potash Potassium hydrate
Sumformula of the chemical	HKO
Molecular weight	56.11
LD50 values to mammals in oral exposure, mg/kg	365 orl-rat (Sweet 1987)
Other information about mammals	Skin and eye irritation data: skin, human, 50 mg, 24hr, severe; skin, rabbit, 50 mg, 24hr, severe; eye, rabbit, 1 mg, 24hr rinse, moderate; skin, guinea pig, 50 mg, 24hr, severe (Sweet 1987).

Mutagenicity	Mutation data: cytogenetic analysis: rat, Ascites tumor, 1800 mg/kg (Sweet 1987).

1687 • Potassium nitrate 7757-79-1

LC50 values to fishes, mg/l	200	72hr, Poecilia reticulata (Rubin & Elmaraghy 1977)

1688 • Potassium permanganate 7722-64-7

EC50 values to crustaceans, mg/l	0.99 0.5	2d, mbt, Crangonyx pseudogracilis 4d, mbt, Crangonyx pseudogracilis (Martin & Holdich 1986)
LC50 values to fishes, mg/l	3.06 21.6 2.5	96hr, Anguilla rostrata (Hinton & Eversole 1978) 96hr, Anguilla rostrata (Hinton & Eversole 1980) 96hr, Morone saxatilis (Kemp et al. 1973)

1689 • Potassium ricinoleate 749-23-0

Other information about water organisms	Ictalurus puncatus, 0.8 mg/l, 150 d, change in biomass in a defined area (Tucker & Lloyd 1987).

1690 • Potassium sulfate 7778-80-5

Synonyms	Sulfuric acid, dipotassium salt	
Sumformula of the chemical	04S.2K	
Molecular weight	174.26	
LD50 values to mammals in oral exposure, mg/kg	6600	orl-rat (Sweet 1987)
LDLo values to mammals in oral exposure, mg/kg	800	orl-wmn (Sweet 1987)
LDLo values to mammals in non-oral exposure, mg/kg	3000	scu-gpg (Sweet 1987)
LC50 values to crustaceans, mg/l	1180	96hr, 10 °C, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	2380	96hr, 10 °C, Alburnus alburnus (Linden et al. 1979)

PQR

1691 • Potassium thiocyanate 333-20-0

LC50 values to crustaceans, mg/l	2.79–33.5	4d, Daphnia magna (Watson & Maly 1987)

1692 • Potassium-N-hydroxymethyl-N-methyldithiocarbamate 51026-28-9

Use	Slimicide.	
LOEC values to fishes, mg/l	0.4–0.5	srv, juv, act, Branchydanio rerio (Björndal et al.1984)

1693 • Primene JM-T * 69225-84-9

Chemicals in the product	Product is a mixture of long chained, aliphatic ammonium salts of chloromethylphosphoric acid.	
LC50 values to fishes, mg/l	0.47	96hr, Branchydanio rerio (Dave et al. 1981)
	1.2–5.3	120hr, Salmo gairdneri, juv. (Dave et al. 1979)
	0.25–0.45	96hr, Salmo gairdneri (Dave & Lindman 1978)

1694 • Prometone 1610-18-0

Synonyms	2,4-Bis(isopropylamino)-6-methoxy-s-triazine	
Use	Herbicide.	
Effects on plants	Soil was amended to give 2.0 ppm by weight of soil of prometone → atrazine-susceptible lamb's-quarters (Chenopodium album L.) were killed soon after germination and emergence (Jensen et al. 1977). 3.0 kg prometone/ha was applied with a sprayer following seeding (preemergence) to lamb's-quarters (Chenopodium album L.) → atrazine-susceptible plants (seeds) were killed and there was a decrease in shoot growth and plant number of atrazine-resistant plants (Jensen et al. 1977).	
EC50 values to algae, mg/l	0.1	pht, 10d, Phaeodactylum tricornutum
	0.25	rpd, 10d, Phaeodactylum tricornutum (Walsh 1972)

1695 • Prometryne 7287-19-6

Synonyms	2,4-Bis(isopropylamino)-6-(methylthio)-s-triazine N,N'-Di-isopropyl-6-methylthio-1,3,5-triazine-2,4-diyldiamine	
Use	Active ingredient in herbicides.	
Effects on plants	Soil was amended to give 2.0 ppm by weight of soil of prometryn → atrazine-susceptible lamb's-quarters (Chenopodium album L.) were killed soon after germination and emergence (Jensen et al. 1977). Vicia sativa (L.) was subjected to preemergence sprays of prometryn (1.0 kg/ha) → a significant decrease in mean leaf area (Prakash et al. 1978).	
LC50 values to crustaceans, mg/l	> 40	act, Daphnia pulex (Nishiuchi & Hashimoto 1967)
LC50 values to fishes, mg/l	2.5	96hr, Salmo gairdneri
	10	96hr, Lepomis macrochirus (Pesticide Manual 1983)
	5.2	96hr, Cyprinus carpio (Nishiuchi & Hashimoto 1967)

1696 • Propachlor 1918-16-7

Synonyms	2'-Chloro-N-isopropylacetanilide	
Use	Active ingredient in herbicides.	
Molecular weight	211.71	
Log soil sorption coefficient, log Kom	2.42	(Sabljic 1987)
Half-life in soil, days	7	(Li et al. 1990)

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LD50 values to mammals in oral exposure, mg/kg	710 290	orl-rat orl-mus (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	380	skn-rbt (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	512	orl-dck (Lewis & Sweet 1984)
Effects on plants	4.37 kg propachlor/ha a.i. reduced the fresh weight of weeds at harvest (x = 72). (Roberts & Bond 1975)	
LC50 values to crustaceans, mg/l	7	act, Daphnia magna (Kenaga 1979)
NOEC values to crustaceans, mg/l	1	rpd, schr, Daphnia magna (Macek & Sleight 1977)
LC50 values to fishes, mg/l	0.16 > 1.4 0.17	act, Salmo gairdneri (Kenaga 1979) 96hr, Lepomis macrochirus 96hr, Salmo gairdneri (Pesticide Manual 1983)
NOEC values to fishes, mg/l	0.17	rpd, chr, Pimephales promelas (Macek & Sleight 1977)

1697 • (S)-(+)-Propane-1,2-diol 4254-15-3

Sumformula of the chemical	C3H8O2	
Water solubility, mg/l	> 100000	(MITI 1992)
Melting point, °C	-59	(MITI 1992)
Boiling point, °C	188.2	760 mmHg (MITI 1992)
Total degradation in water	Biodegradation: 87–92% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

1698 • Propanil 709-98-8

Synonyms	N-(3,4-Dichlorophenyl)-propionamide 3',4'-Dichloropropionanilide	
Use	Herbicide.	
Molecular weight	218.09	
Vapour pressure, mmHg	0.00009	60 °C
Water solubility, mg/l	50–225, room temperature	
Melting point, °C	90.6–91.6	
LD50 values to mammals in oral exposure, mg/kg	560 360	orl-rat orl-mus (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	4830	skn-rbt (Lewis & Sweet 1984)

Effects on plants	Green foxtail plants (Setaria viridis) sprayed with 0.5 kg propanil/ha at the 4-leaf stage were markedly reduced in size (a greenhouse experiment) (Hunter 1980). Incubation of segments of barley coleoptile and Sesbania exaltata hypocotyls in 1% sucrose containing 5 ppm propanil inhibited protein synthesis by 8 and 14%, respectively (Mann et al. 1965).
EC50 values to microorganism, mg/l	82.3 DIDHA, ethanol (Bitton et al. 1986) 11.6 DIDHA, DMSO (Bitton et al. 1986)
EC50 values to algae, mg/l	0.051–0.109 0.13d, oxygen production (Tucker 1987)
LC50 values to crustaceans, mg/l	16 96hr, Gammarus fasciatus (Sanders 1970) > 40 act, Daphnia pulex (Hashimoto & Nishiuchi 1981)
EC50 values to crustaceans, mg/l	4.8 rpd, act, Daphnia magna (Martin 1968)
LC50 values to fishes, mg/l	3.8 96hr, Ictalurus punctatus (McCorkle et al. 1977) 8.6 96hr, Pimephales promelas (Call et al. 1983) 13 48hr, Cyprinus carpio 14 48hr, Carassius auratus (Hashimoto & Nishiuchi 1981) 5.8 72hr, Lepomis cyanellus (Davey et al. 1976)
LOEC values to fishes, mg/l	0.0006 grw, schr, Pimephales promelas (Call et al. 1983)
NOEC values to fishes, mg/l	0.0004 grw, schr, Pimephales promelas (Call et al. 1983)

1699 • n-Propanol

71-23-8

Synonyms	Propyl alcohol
Sumformula of the chemical	C3H8O
Use	Solvent.
Odour	Quality: sweet, alcohol Hedonic tone: pleasant Threshold odour concentration absolute: < 0.03 ppm 50% recognition: 0.08 ppm 100% recognition: 0.13 ppm Odour index 100% recognition: 246 625 (Hellman & Small 1974).
Molecular weight	60.11
Melting point, °C	-126.5
Boiling point, °C	97.4
Log octanol/water coefficient, log Pow	0.25 (Sangster 1989)
Henry's law constant, Pa x m^3/mol	0.9253 calc. (Yaws et al. 1991)
Volatilization	Relative volatility (nBuAc=1) = 0.94
LD50 values to mammals in oral exposure, mg/kg	1870 orl-rat
Maximum longterm immission concentration in air for plants, mg/m^3	50 VDI 2306

PQR

Maximum longterm immission concentration in air for plants, ppm	20	VDI 2306
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 2700 mg/l (Bringmann & Kühn 1980a).	
EC50 values to microorganism, mg/l	8700 19091	15 min Microtox (Hermens et al. 1985) Biodegration inhibition (Vaishnav 1986)
NOEC values to algae, mg/l	2000	rpd, schr, Selenastrum caprinornutum (Slooff et al. 1983)
LC50 values to crustaceans, mg/l	7080 3025 5820 2300 2500 1000	48hr, Daphnia magna 48hr, Daphnia pulex 48hr, Daphnia cucullata (Canton & Adema 1978) 96hr, 21 °C, Nitocra spinipes (Linden et al. 1979) 48hr, Asellus aquaticus (Slooff 1983) 48hr, Gammarus pulex (Slooff 1983)
LC50 values to fishes, mg/l	3200 3000–4000	48hr, Salmo gairdneri (Slooff et al. 1983) 96hr, 10 °C, Alburnus alburnus (Linden et al. 1979)
Other information about water organisms	LOEC 38 mg/l, rpd, scht, Entosiphon sulcatum (Bringmann & Kühn 1980a). LC50, 48hr, 9200 mg/l, Tubificidae LC50, 48hr, 2350 mg/l, Chironomus gr. thummi LC50, 48hr, 1400 mg/l, Erpobdella octoculata LC50, 48hr, 6500 mg/l, Lymnaea stagnalis LC50, 48hr, 4700 mg/l, Dugesia cf. lugubris LC50, 48hr, 6800 mg/l, Hydra oligactis LC50, 48hr, 2000 mg/l, Corixa punctata LC50, 48hr, 4200 mg/l, Ischura elegans LC50, 48hr, 1520 mg/l, Nemoura cinerea LC50, 48hr, 3110 mg/l, Cloeon dipterum (Slooff 1983) Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 3100 mg/l protozoa (Entosiphon sulcatum): 38 mg/l (Bringmann & Kühn 1980a)	

1700 • Propargyl alcohol 107-19-7

Synonyms	Ethynylcarbinol 2-Propyn-1-ol 1-Propyne-3-ol 3-Propynol 2-Propynyl alcohol	
Sumformula of the chemical	C3H4O	
Log octanol/water coefficient, log Pow	-0.38	(Sangster 1989)
LOEC values to algae, mg/l	18	rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
Other information about water organisms	LOEC 17 mg/l, rpd, schr, Entosiphon sulcatum (Bringmann & Kühn 1980a).	

1701 • Propene

115-07-1

Synonyms	Methylethene Methylethylene 1-Propene Propylene
Sumformula of the chemical	C3H6
Odour	Quality: aromatic Hedonic tone: neutral to pleasant Threshold odour concentration absolute: 22.5 ppm 50% recognition: 67.6 ppm 100% recognition: 67.6 ppm Odour index 100% recognition: 14 792 (Hellman & Small 1974).
Molecular weight	42.09
Henry's law constant, Pa x m³/mol	20650 calc. (Yaws et al. 1991)
Carcinogenicity	NTP carcinogenesis studies (inhalation); no evidence: mouse, rat (Sweet 1987).

1702 • Propeneoxide

75-56-9

Synonyms	1,2-Epoxypropane Propyleneoxide Epoxypropane
Sumformula of the chemical	C3H6O
Use	Solvent.
Odour	Quality: sweet Hedonic tone: neutral to pleasant Threshold odour concentration absolute: 9.9 ppm 50% recognition: 35.0 ppm 100% recognition: 35.0 ppm Odour index 100% recognition: 16 600 (Hellman & Small 1974).
Water solubility, mg/l	> 100 000 (MITI 1992)
Melting point, °C	< -10 (MITI 1992)
Boiling point, °C	34.2 35 (MITI 1992)
Log octanol/water coefficient, log Pow	0.03 (Sangster 1989)
Chemical oxygen demand, g O2/g	1.77 5 days (Bridie et al. 1979)
Biochemical oxygen demand, g O2/g	0.17 5 days (Bridie et al. 1979)
Total degradation in water	Biodegradation: 93–98% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

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LD50 values to mammals in oral exposure, mg/kg	930	orl-rat
LC50 values to fishes, mg/l	141 215 170	96hr, Gambusia affinis 96hr, Lepomis macrochirus (Crews 1974) 24hr, Carassius auratus (Bridie et al. 1979)

1703 • β-Propiolactone 57-57-8

Synonyms	Propiolactone 2-Oxetanone
Sumformula of the chemical	C3H4O2
EINECS-number	2003401
Water solubility, mg/l	> 100000 (MITI 1992)
Melting point, °C	-33.4 (MITI 1992)
Photochemical degradation in air	Photo oxidation half-life in air: 7.5d–75d, based upon estimated rate constant for reaction with hydroxyl radicals in air (Howard 1991).
Hydrolysis in water	First-order hydrolysis half-life: 0.058hr–3.4hr, based on measured hydrolysis rate constant in water at 25 °C (Howard 1991).
Half-life in air, days	7.5d–75d, based upon estimated photo oxidation half-life in air (Howard 1991)
Half-life in soil, days	0.002–0.142d = 0.058–3.4hr, based on measured hydrolysis rate constant in water at 25 °C (Howard 1991)
Half-life in water, days	0.002–0.142d= 0.058–3.4hr, in surface water, based on measured hydrolysis rate constant in water at 25 °C; 0.002–0.142d= 0.058–3.4hr, in ground water, based on measured hydrolysis rate constant in water at 25 °C (Howard 1991)
Aerobic degradation in water	Aerobic half-life: 1d–7d, scientific judgement based upon unacclimated aerobic aqueous screening test data (Howard 1991).
Anaerobic degradation in water	Anaerobic half-life: 4d–28d, scientific judgement based estimated aqueous aerobic biodegradation half-life (Howard 1991).
Total degradation in water	Biodegradation: 76–81% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

1704 • Propionaldehyde 123-38-6

Synonyms	Methylacetaldehyde Propanal

Odour	Quality: sweet, ester Hedonic tone: pleasant Threshold odour concentration absolute: 0.009 ppm 50% recognition: 0.040 ppm 100% recognition: 0.080 ppm Odour index 100% recognition: 4 346 000 (Hellman & Small 1974).	
Water solubility, mg/l	> 100000 (MITI 1992)	
Melting point, °C	-81	(MITI 1992)
Boiling point, °C	47.5–49	(MITI 1992)
Log octanol/water coefficient, log Pow	0.59	(Sangster 1989)
Total degradation in water	Biodegradation: 91–97% by BOD period 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
LC50 values to fishes, mg/l	130 100	96hr, Lepomis macrochirus 96hr, Menidia audens (Dawson et al. 1977)

1705 • Propionic acid 79-09-4

Synonyms	Methylacetic acid	
Sumformula of the chemical	C3H6O2	
Odour	Quality: sour Hedonic tone: unpleasant Threshold odour concentration absolute: 0.028 ppm 50% recognition: 0.034 ppm 100% recognition: 0.034 ppm Odour index 100% recognition: 91 500 (Hellman & Small 1974).	
pKa	4.87	(Sangster 1989)
Log octanol/water coefficient, log Pow	0.33	(Sangster 1989)
LC50 values to crustaceans, mg/l	50	48hr, Daphnia magna (Dowden & Bennet 1965)
LC50 values to fishes, mg/l	188	24hr, Lepomis macrochirus (Dowden & Bennett 1965)

1706 • Propiophenone 93-55-0

Sumformula of the chemical	C9H10O	
Log octanol/water coefficient, log Pow	2.19	(Sangster 1989)

PQR

1707 • n-Propylacetate 109-60-4

Synonyms	1-Propylacetate	
Sumformula of the chemical	C5H10O2	
Use	Solvent.	
Odour	Quality: sweet, ester Hedonic tone: pleasant Threshold odour concentration absolute: 0.05 ppm 50% recognition: 0.15 ppm 100% recognition: 0.15 ppm Odour index 100% recognition: 218 666 (Hellman & Small 1974).	
Boiling point, °C	101.6	
Log octanol/water coefficient, log Pow	1.24	(Sangster 1989)
LD50 values to mammals in oral exposure, mg/kg	9800	orl-rat
LOEC values to algae, mg/l	26	rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
Other information about water organisms	LOEC 97 mg/l, rpd, schr, Entosiphon sulcatum (Bringmann & Kühn 1980a).	

1708 • n-Propylbenzene 103-65-1

Sumformula of the chemical	C9H12	
Log octanol/water coefficient, log Pow	3.69	(Sangster 1989)

1709 • s-Propyldipropyldithiocarbamate 1929-77-7

Use	Herbicide.	
LC50 values to crustaceans, mg/l	0.24 1.1	48hr, Cypridopsis vidua 48hr, Daphnia magna (Sanders 1970)

PQR

1710 • Propyleneglycol 57-55-6

Synonyms	1,2-Propanediol	
Sumformula of the chemical	C3H8O2	
Use	Solvent.	
Molecular weight	76.11	
Vapour pressure, mmHg	0.08	at 20 °C (Weber et al. 1981)
Boiling point, °C	189	
Log octanol/water coefficient, log Pow	-0.92	(Hansch & Leo 1985)
Henry's law constant, Pa x m^3/mol	0.0012	(Simmons et al. 1976)

Volatilization	Relative volatility (nBuAc=1) = 0.010 The value of the Henry's Law constant indicates that 1,2-propanediol is essentially not volatile from water (Lyman et al. 1982).
Mobility	The complete miscibility in water and low Kow of 1,2-propanediol is indicative of very high mobility in soil (Howard 1990). Miscible (Merck Index 1983).
Chemical oxygen demand, g 02/g	1.63 5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	1.08 5 days (Bridie et al. 1979)
Other information about degradation	Standard dilution BOD water, 5-day 64% BODT, sewage inocula (Bridie et al. 1979). Nutrient broth, 100% degradation in 4 days (aerobic conditions), 100% degradation in 4–9 days (anaerobic conditions), activated sludge or digester sludge inocula, no significant degradation in sterile controls (Kaplan et al. 1982). Standard dilution BOD water, 5-day 62% BODT, 20-day 79% BODT, sewage inocula; syntetic seawater dilution, 5-day 55% BODT, 20-day 83% BODT, raw wastewater inocula (Price et al. 1974). Sewage die-away, 74.5% BODT in 5 days (Wagner 1976). 1,2-propanediol has been found to be degradable via anaerobic biotechnology (Howard 1990). Standard dilution BOD water, 5-day 26.6% BODT; seawater dilution, 5-day 59.5% BODT (Takemoto et al. 1981).
LD50 values to mammals in oral exposure, mg/kg	21000
EC50 values to microorganism, mg/l	34800 Microtox (Tarkpea et al. 1986)
LC50 values to fishes, mg/l	> 5000 24hr, Carassius auratus (Bridie et al. 1979)

1711 • Propylenetetramer 6842-15-5

Water solubility, mg/l	< 100	(MITI 1992)
Melting point, °C	< -10	(MITI 1992)
Boiling point, °C	183–204	(MITI 1992)
Log octanol/water coefficient, log Pow	> 3.84	(MITI 1992)
Total degradation in water	Biodegradation: 6–9% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	1960–4100 796–2780	8w, Cyprinus crpio, conc 0.1 mg/l 8w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
LC50 values to fishes, mg/l	7.92	48hr, Oryzias latipes (MITI 1992)

PQR

1712 • Propyzamide 23950-58-5

Use	Herbicide.
Effects on plants	Propyzamide reduced germination of dodder (Cuscuta australis) seeds by 42% and reduction of stem elongation was 75% at a concentration of 0.010 mg/ml (seeds/seeds with shoots were placed to Petri dishes on filter paper where herbicide solution was added). There was a decrease in seedling emergence and height of dodder sown in a silt loam soil treated with 2.0 kg propyzamide/ha (Giannopolitis 1979).

1713 • Prothiocarb 19622-08-3

Synonyms	S-Ethyl(3-dimethylaminopropyl)thiocarbamate	
Use	Fungicide.	
LC50 values to fishes, mg/l	328	96hr, Salmo gairdneri
	258	96hr, Lepomis macrochirus (Pesticide Manual 1983)

1714 • Proxel PL * 2634-33-5

Active ingredients	1,2-benzisothiazolene-3-one * 33%	
Use	Pesticide, slimicide.	
LC50 values to crustaceans, mg/l	25	96hr, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	10	96hr, Alburnus alburnus (Linden et al. 1979)

1715 • Pydraul 50 E 66594-31-8

Synonyms	Pydraul 50E	
Chemicals in the product	Phosphate ester	
LC50 values to fishes, mg/l	0.67	96hr, Salmo gairdneri
	2.8	96hr, Lepomis macrochirus
	1.7	96hr, Pimephales promelas
	1.3	10 d, Pimephales promelas (Nevins & Johnson 1978)

PQR

1716 • Pyrazon 1698-60-8

Synonyms	5-Amino-4-chloro-2-phenyl-3(2H)-pyridazinone
Use	Herbicide.
Effects on plants	1.0 kg pyrazon/ha was applied with a sprayer following seeding (preemergence) to lamb's-quarters (Chenopodium album L.) → decrease in shoot growth of atrazine-susceptible plants (Jensen et al. 1977).

1717 • Pyrazoxon 108-34-9

Other information about mammals	LDfr = 12.5 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).	
LD50 values to birds in oral exposure, mg/kg	40	orl-Sturnus vulgaris (Schafer et al. 1983)

1718 • Pyrene

129-00-0

Synonyms	Benzo(def)phenanthrene
Sumformula of the chemical	C16H10
Molecular weight	202.26
Log octanol/water coefficient, log Pow	5.18 observed (Chin et al. 1986) 5.18 (Schwarzenbach & Westall 1981) 5 (Sangster 1989)
Log organic C/water coefficient, log Pcw	4.92 exptl (Schwarzenbach & Westall 1981) 4.22 calcd (Schwarzenbach & Westall 1981)
Other information about degradation	Degradation of pyrene: (see table below)
Effects on arthropods	LC50, 1 d: Aedes aegypti, 0.035 mg/l; Aedes taeniorhynchus, 0.060 mg/l; Culex quinquefasciatus, 0.037 mg/l (Borovsky et al. 1987).
LC50 values to fishes, mg/l	0.0026 96hr, Gambusia affinis (Miura & Takahashi 1976)
Other information about water organisms	Lethal threshold concentration (LT50): Daphnia magna, 0.0057 mg/l. 0.14d (Newsted & Giesy 1987); Pimephales promelas, 0.0256 mg/l, 0.13d (Oris & Giesy 1987).

Degradation of pyrene:

ENVIRONMENT	*INIT CONC. mg/l*	*REDOX-COND.*	*TEMP. °C*	*DEGRADATION %/day*	*REF.*
water	5	aerobic	25	71/7	a
water	10	aerobic	25	11/7	a
water (adapted)	5	aerobic	25	100/7	a
water (adapted)	10	aerobic	25	0/7	a
sea water	0.365	aerobic	10	85/12	b
soil	3.1	aerobic	–	19/10	c

a) Tabak et al. 1981
b) McKenzie & Hughes 1976
c) Groenewegen & Stolp 1976 (Anon. 1987b).

1719 • Pyrethrin

8003-34-7

Use	Active ingredient in insecticides.
LD50 values to mammals in oral exposure, mg/kg	200 orl-rat 250 orl-mam (Lewis & Sweet 1984)
LC50 values to crustaceans, mg/l	0.025 48hr, Daphnia pulex (Sanders & Cope 1966) 0.011 96hr, Gammarus fasciatus (Sanders 1972) 0.025 act, Daphnia pulex (Kenaga 1979)
LC50 values to fishes, mg/l	0.054 act, Salmo gairdneri 0.07 act, Lepomis macrochirus (Kenaga 1979) 0.049 96hr, Lepomis macrochirus 0.023 96hr, Oncorhynchus kisutch (Mauck & Olson 1976) 0.056 24hr, Salmo gairdneri (Könemann 1979)

PQR

1720 • Pyridine

110-86-1

Sumformula of the chemical	C5H5N	
Use	Solvent.	
Molecular weight	79.1	
Melting point, °C	-42	
Boiling point, °C	115.5	
pKa	5.21	(Sangster 1989)
Log octanol/water coefficient, log Pow	0.65	(Sangster 1989)
Volatilization	Relative volatility (nBuAc=1) = 1.51	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	891	orl-rat
LD50 values to birds in oral exposure, mg/kg	> 1000 > 1000 > 1000 > 1000	orl-Agelaius phoeniceus orl-Sturnus vulgaris orl-Coturnix coturnix orl-Passer domesticus (Schafer et al. 1983)
Maximum longterm immission concentration in air for plants, mg/m³	0.7	VDI 2306
Maximum longterm immission concentration in air for plants, ppm	0.2	VDI 2306
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 340 mg/l (Bringmann & Kühn 1980a).	
EC50 values to microorganism, mg/l	737	15 min Microtox (Kaiser and Ribo 1985)
LOEC values to algae, mg/l	28	rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
NOEC values to algae, mg/l	50	rpd, schr, Selenastrum capricornutum (Slooff et al. 1983)
LC50 values to crustaceans, mg/l	1350 575 2470 220 182	48hr, Daphnia magna 48hr, Daphnia pulex 48hr, Daphnia cucullata (Canton & Adema 1978) 48hr, Asellus aquaticus (Slooff 1983) 48hr, Gammarus pulex (Slooff 1983)

PQR

LC50 values to fishes, mg/l	1350	24hr, Gambusia affinis (Wallen et al. 1957)
	330	48hr, Oryzias latipes (Tonogai et al. 1982)
	560	48hr, Salmo gairdneri (Slooff et al. 1983)
	1.3	1d, Oncorhynchus gorbuscha
	1.1	4d, Oncorhynchus gorbuscha
	4	1d, Oncorhynchus keta
	3.7	4d, Oncorhynchus keta
	4.3	1d, Oncorhynchus kisutch
	3.8	4d, Oncorhynchus kisutch
	6.9	1d, Oncorhynchus nerka
	6.3	4d, Oncorhynchus nerka
	3.2	1d, Oncorhynchus tshawytscha
	2.9	4d, Oncorhynchus tshawytscha
	4.6	1d, Salmo gairdneri
	4.6	4d, Salmo gairdneri (Wan et al. 1987)
Other information about water organisms	LOEC 3.5 mg/l, rpd, schr, Entosiphon sulcatum (Bringmann & Kühn 1980a). LC50, 48hr, 1300 mg/l, Tubificidae LC50, 48hr, 229 mg/l, Chironomus gr. thummi LC50, 48hr, 2400 mg/l, Erpobdella octoculata LC50, 48hr, 350 mg/l, Lymnaea stagnalis LC50, 48hr, 1900 mg/l, Dugesia cf. lugubris LC50, 48hr, 1150 mg/l, Hydra oligactis LC50, 48hr, 30 mg/l, Corixa punctata LC50, 48hr, 410 mg/l, Ischura elegans LC50, 48hr, 254 mg/l, Nemoura cinerea LC50, 48hr, 165 mg/l, Cloeon dipterum (Slooff 1983) Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 120 mg/l protozoa (Entosiphon sulcatum): 3.5 mg/l (Bringmann & Kühn 1980a)	

1721 • 2-Pyridine carboxaldehyde 1121-60-4

Other information about water organisms	Tetrahymena pyriformis, EC50, grw, 2.5 d, 131.2 mg/l (Schultz et al. 1987).

1722 • 3-Pyridine carboxaldehyde 500-22-1

LD50 values to birds in oral exposure, mg/kg	> 1000	orl-Agelaius phoeniceus
	> 1000	orl-Sturnus vulgaris
	> 1000	orl-Coturnix coturnix
	> 1000	orl-Passer domesticus (Schafer et al. 1983)
Other information about water organisms	Tetrahymena pyriformis, EC50, grw, 2.5 d, 134.4 mg/l (Schultz et al. 1987).	

1723 • Pyridine-2,5-dicarboxylic acid 100-26-5

Sumformula of the chemical	C7H5NO4
EINECS-number	2028342

PQR

Water solubility, mg/l	15100 (MITI 1992)
Bioconcentration factor, fishes	< 0.3–0.9 6w, Cyprinus carpio, conc 2 mg/l < 2.9–8.6 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 1000 48hr, Oryzias latipes (MITI 1992)

1724 • Pyridine-2,5-dicarboxylic acid dipropyl 136-45-8

Synonyms	2,5-Pyridinedicarboxylic acid, dipropyl ester
Sumformula of the chemical	C13H17N04
EINECS-number	2052459
Boiling point, °C	150 (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
Total degradation in water	Biodegradation: 0% by BOD (hydrolyzed to Pyridine-2,5-dicarboxylic acid) period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

1725 • 2-Pyridinecarbonitrile 100-70-9

Other information about water organisms	Tetrahymena pyriformis, EC50, grw, 2.5 d, 646.7 mg/l (Schultz et al. 1987).

1726 • 3-Pyridinecarbonitrile 100-54-9

Other information about water organisms	Tetrahymena pyriformis, EC50, grw, 2.5 d, 581.6 mg/l (Schultz et al. 1987).

PQR

1727 • 2-Pyridinecarboxylic acid 98-98-6

LD50 values to birds in oral exposure, mg/kg	178 orl-Agelaius phoeniceus 750 orl-Sturnus vulgaris 562 orl-Coturnix coturnix 178 orl-Passer domesticus (Schafer et al. 1983)
Other information about water organisms	Tetrahymena pyriformis, EC50, grw, 2.5 d, 104.6 mg/l (Schultz et al. 1987).

1728 • 3-Pyridinecarboxylic acid 59-67-6

Other information about water organisms	Tetrahymena pyriformis, EC50, grw, 2.5 d, 2792.9 mg/l (Schultz et al. 1987).

1729 • 2,6-Pyridinedicarboxylic acid 499-83-2

Sumformula of the chemical	C7H5O4N
Water solubility, mg/l	> 10000 (MITI 1992)
Melting point, °C	236–237.5 (MITI 1992)
Total degradation in water	Biodegradation: 71–87% (NO2) by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

1730 • 2-Pyridinemethanol 586-98-1

Synonyms	2-Pyridylcarbinol
LD50 values to birds in oral exposure, mg/kg	750 orl-Agelaius phoeniceus > 1000 orl-Sturnus vulgaris 1000 orl-Coturnix coturnix 100 orl-Passer domesticus (Schafer et al. 1983)
Other information about water organisms	Tetrahymena pyriformis, EC50, grw, 2.5 d, 3099.9 mg/l (Schultz et al. 1987).

1731 • 3-Pyridinemethanol 100-55-0

Synonyms	Nicotinyl alcohol
LD50 values to birds in oral exposure, mg/kg	> 1000 orl-Agelaius phoeniceus > 1000 orl-Sturnus vulgaris > 1000 orl-Coturnix coturnix > 1000 orl-Passer domesticus (Schafer et al. 1983)
Other information about water organisms	Tetrahymena pyriformis, EC50, grw, 2.5 d, 3166.2 mg/l (Schultz et al. 1987).

1732 • 1-(3-Pyridyl)-2-nitropropene 3156-53-4

Other information about mammals	LDfr = 86.7 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

1733 • Pyridylmethyl(methylthiophenyl) carbamate 51594-86-6

Other information about mammals	ALD = 22.3–31.7 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987).

PQR

1734 • 3-Pyridylmethyl-N-4'-nitrophenylcarbamate

51594-83-3

Other information about mammals	ALD = 26.0–34.5 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987).

1735 • Pyrogallol

87-66-1

Synonyms	1,2,3-Trihydroxybenzene 1,2,3-Benzenetriol	
LD50 values to birds in oral exposure, mg/kg	75	orl-Agelaius phoeniceus (Schafer et al. 1983)
LC50 values to fishes, mg/l	18	48hr, Carassius auratus (McKee & Wolf 1963)

1736 • Pyrrole

109-97-7

Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LD50 values to birds in oral exposure, mg/kg	> 100	orl-Agelaius phoeniceus (Schafer et al. 1983)

1737 • 2-Pyrrolidone

616-45-5

LD50 values to birds in oral exposure, mg/kg	> 98	orl-Agelaius phoeniceus (Schafer et al. 1983)
NOEC values to algae, mg/l	100	rpd, schr, Selenastrum capricornutum (Verschueren 1983)
LC50 values to crustaceans, mg/l	3.4	act, Daphnia magna (Verschueren 1983)

1738 • Quinalphos

13593-03-8

Synonyms	O,O-Diethyl-O-(2-quinoxalinyl)phosphorothioate	
Molecular weight	298.32	
LD50 values to mammals in oral exposure, mg/kg	26	orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	300	skn-rat (Lewis & Sweet 1984)
LC50 values to mammals in inhalation exposure, mg/m³	175	ihl-rat (Lewis & Sweet 1984)
LC50 values to crustaceans, mg/l	0.461 1.55	96hr, Macrobrachium lamarrei (Omkar & Shukla 1985) 96hr, Saccobranchus fossilis (Verma et al. 1978)
LC50 values to fishes, mg/l	3.45 0.17	48hr, Macropodus cupanus 48hr, Aplocheilus lineatus (Jakob et al. 1982)
Other information about water organisms	LC100 (96hr), 6.91 mg/l, Sarotheredon aureus (Mustafa et al. 1982).	

PQR

1739 • Quinoline 91-22-5

Sumformula of the chemical	C9H7N	
State and appearance	Colourless liquid.	
Molecular weight	129.17	
Vapour pressure, mmHg	1	59.7 °C
Water solubility, mg/l	5000	(MITI 1992)
Melting point, °C	-15	(MITI 1992)
Boiling point, °C	237.7	(MITI 1992)
pKa	4.87	(Sangster 1989)
Log octanol/water coefficient, log Pow	2.03	(Sangster 1989)
Total degradation in water	Biodegradation: 0.2% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	0.1–2.5 1.0–3.8	6w, Cyprinus carpio, conc 0.8 mg/l 6w, Cyprinus carpio, conc 0.08 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	331	orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	540	skn-rbt (Lewis & Sweet 1984)
LC50 values to crustaceans, mg/l	35	48hr, Daphnia magna (Millemann et al.1984)
LC50 values to fishes, mg/l	11.5 0.44 10.8 11 > 10.8 1.77 84	27 d, Salmo gairdneri (Millemann et al. 1984) 96hr, Pimephales promelas (Millemann et al. 1984) 0d, embryo-larval, Salmo gairdneri 4d, embryo-larval, Salmo gairdneri 0d, embryo-larval, Micropterus salmoides 4d, embryo-larval, Micropterus salmoides (Black et al. 1983) 48hr, Oryzias latipes (MITI 1992)

1740 • Quinoline-2-carboxylic acid 93-10-7

Synonyms	2-Quinoline carboxylic acid Quinaldic acid	
Sumformula of the chemical	C10H7NO2	
EINECS-number	2022183	
Water solubility, mg/l	> 1000	(MITI 1992)
Melting point, °C	157	(MITI 1992)

PQR

Total degradation in water	Biodegradation: 81% (NO2) by BOD period: 14 d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

1741 • Quintozene

82-68-8

Synonyms	Pentachloronitrobenzene	
Use	Active ingredient in fungicides.	
EC50 values to microorganism, mg/l	3.8	Microtox, Kaiser and Ribo 1985
Other information about water organisms	LOEC	> 10 mg/l, Colpidium campylum (Dive et al. 1980).

1742 • R-40244

61213-25-0

Synonyms	1-(m-Trifluoromethylphenyl)-3-chloro-4-chloromethyl-2-pyrrolidone
Use	Herbicide.
Effects on plants	Wheat (Triticum aestivum L.) and corn (Zea mays L.) seeds were imbided for 6 hours in solution containing 0.032 mmol/l (w/v) of the herbicide. The imbedded seeds were sown. After 6 days of growth seedlings were collected —a decrease in chlorophyll content (chlorotic development), and an inhibitory effect on the growth in shoot length (Devlin et al. 1979).

1743 • RE 5454

15942-48-0

Other information about mammals	ALD = 42.0 mg/l, act, orl, deer mouse (Virtanen & Nuuja 1987).	
LD50 values to birds in oral exposure, mg/kg	9 16	orl-Agelaius phoeniceus orl-Sturnus vulgaris (Schafer et al. 1983)

1744 • Reactive Black-5

17095-24-8

Sumformula of the chemical	C26H25N5019S6.4Na	
Water solubility, mg/l	> 10000	(MITI 1992)
Bioconcentration factor, fishes	< 1.1 < 11	6w, Cyprinus carpio, conc 2 mg/l 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 1000	48hr (MITI 1992)

1745 • Resmethrin

10453-86-8

Use	Insecticide.	
LD50 values to birds in oral exposure, mg/kg	75 > 100	orl-Agelaius phoeniceus orl-Passer domesticus (Schafer et al. 1983)
LC50 values to fishes, mg/l	0.00027 0.00051	96hr,hrd, Salmo gairdneri 96hr,hrd, Perca flavescens (Mauck & Olson 1976)

1746 • Resorcinol

108-46-3

Synonyms	m-Hydroxyphenol m-Hydroquinone 1,3-Dihydroxybenzene 3-Hydroxyphenol m-Dihydroxybenzene m-Benzenediol 1,3-Benzenediol m-Dioxybenzene Resorcin Resorcine 3-Hydroxycyclohexadien-1-one	
Sumformula of the chemical	C6H6O2	
Molecular weight	110.12	
Melting point, °C	111	(MITI 1992)
Boiling point, °C	281.4	(MITI 1992)
Total degradation in water	Biodegradation: 66.7% by BOD period: 14d substance 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	301	orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	3360 215 213	skn-rbt (Lewis & Sweet 1984) ipr-mus scu-mus (Sweet 1987)
LDLo values to mammals in oral exposure, mg/kg	29 301	orl-hmn (Lewis & Sweet 1984) orl-rat (Sweet 1987)
LDLo values to mammals in non-oral exposure, mg/kg	400 250 700 110 400 340	scu-rat (Lewis & Sweet 1984) ips-mus (Lewis & Sweet 1984) ivn-dog (Lewis & Sweet 1984) scu-cat (Lewis & Sweet 1984) scu-gpg (Lewis & Sweet 1984) scu-mus (Lewis & Sweet 1984)
TDLo values to mammals in non-oral exposure, mg/kg	4800	skn-mus (Lewis & Sweet 1984)

PQR

Carcinogenicity	TDLo 4800 mg/kg/12W-I; tumorigenic (Equivocal tumorigenic agent by RTECS criteria); skin and appendages (Sweet 1987).
Effects on amphibia	LD50 270 mg/kg, parenteral, frog (Sweet 1987).
LC50 values to fishes, mg/l	57 48hr, Carassius auratus (McKee & Wolf 1963) 53 96hr, Pimephales promelas (Curtis et al. 1979) 100 96hr, Pimephales promelas (DeGraeve et al. 1980) 108.6 Tilapia mossambica (Devi & Sastry 1987)
Other information about water organisms	Tetrahymena pyriformis; EC50, grw, 2d days: 542.66 mg/l (Schultz 1987).

1747 • Rhodamine

81-88-9

Synonyms	2-(3-Diethylimino-6-diethylamino-3H-xanthen-9-yl)benzoic acid chloride
Water solubility, mg/l	10000 (MITI 1992)
Melting point, °C	172–176 (MITI 1992)
Log octanol/water coefficient, log Pow	1.9–2.0 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.2 6w, Cyprinus carpio, conc 0.1 mg/l < 1.7 6w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
LC50 values to fish, mg/l	12 48hr, Oryzias latipes (Tonogoi et al. 1982) 33.9 48hr, Oryzias latipes (MITI 1992)

1748 • Rotenone

83-79-4

Synonyms	Dactinol
Use	Poison for fishes, insecticide, acaricide, active ingredient: Rotenol (5%).
Molecular weight	394.45
Water solubility, mg/l	15 100 °C
Melting point, °C	178–181
Boiling point, °C	210–220
LD50 values to mammals in oral exposure, mg/kg	60 orl-rat (Lewis & Sweet 1984)
Effects on arthropods	Tanytarsus dissimilis, LC50, 2 d, > 0.040 mg/l (Holcombe et al. 1987).
LC50 values to crustaceans, mg/l	0.19 48hr, Simocephalus serrulatus 0.1 48hr, Daphnia pulex (Sanders & Cope 1966) 0.57 act, Daphnia pulex (Hashimoto & Nishiuchi 1981) 0.1 act, Daphnia pulex (Kenaga 1979)
EC50 values to crustaceans, mg/l	0.008 2d, mbt, Daphnia magna (Holcombe et al. 1987)

LC50 values to fishes, mg/l	0.033	48hr, Carassius auratus
	0.032	48hr, Cyprinus carpio (Hashimoto & Nishiuchi 1981)
	0.22	act, Lepomis macrochirus
	0.026	Salmo gairdneri (Kenaga 1979)
	0.044	96hr, Salvelinus fontinalis
	0.033	96hr, Esox lucius
	0.027	96hr, Salmo trutta m. lacustris
	0.046	96hr, Salmo gairdneri
	0.021	96hr, Salmo salar (Martin 1968)
	9.5	24hr, Rasbora heteromorpha
	5.8	48hr,hrd, Salmo gairdneri
	0.47	48hr, sft, Salmo gairdneri (Tooby et al. 1975)
	0.011	4d, Catostomus commersoni
	0.014	4d, Lepomis macrochirus
	0.006	4d, Pimephales promelas
	0.005	4d, Salmo gairdneri (Holcombe et al. 1987)
Other information about water organisms	Aplexa hypnorum, LC50, 4 d, > 0.040 mg/l (Holcombe et al. 1987). Salmo gairdneri, LD50, 0.25 d, 0.305 mg/kg (Erickson & Gingerich 1986).	

1749 • Roundup * 1071-83-6

Active ingredients	Glyphosate as isopropylamine salt * 360 g/kg	
Use	Herbicide.	
EC50 values to microorganism, mg/l	127	Microtox (Tarkpea et al. 1986)
LC50 values to crustaceans, mg/l	5.3	48hr, Daphnia magna (Anon. 1984) (Monsanto)
	22	96hr, Nitocra spinipes (Linden et al. 1979)
EC50 values to crustaceans, mg/l	25.5	4d, mbt, Daphnia pulex (Servizi et al. 1987)
LC50 values to fishes, mg/l	11	96hr, Salmo gairdneri
	9.4	96hr, Pimephales promelas
	14	96hr, Lepomis macrochirus
	16	96hr, Ictalurus punctatus (Anon. 1984) (Monsanto)
	13	96hr, Ictalurus punctatus
	5	96hr, Lepomis macrochirus
	2.3	96hr, Pimephales promelas
	8.3	96hr, Salmo gairdneri (Folmar 1979)
	16	96hr, Alburnus alburnus (Linden et al. 1979)
	25.5	4d, Salmo gairdneri
	28	4d, Salmo gairdneri
	42	4d, Oncorhynchus kisutch
	26.7–28.8	4d, Oncorhynchus nerka (Servizi et al. 1987)

1750 • Salicylaldehyde

90-02-8

Synonyms	Salicylal o-Hydroxybenzaldehyde	
Use	Analytical chemistry, perfumery, synthesis of coumarins, gasoline additives.	
State and appearance	Colourless oily liquid or dark red oil, burning taste.	
Molecular weight	122.1	
Vapour pressure, mmHg	1	33 °C
Melting point, °C	-7	
Boiling point, °C	196	
LD50 values to mammals in oral exposure, mg/kg	520	orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	600	skn-rat (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	> 111	orl-Agelaius phoeniceus (Schafer et al. 1983)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 10 mg/l (Bringmann & Kühn 1980a)	
LOEC values to algae, mg/l	1.6	rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
NOEC values to algae, mg/l	5.5	rpd, schr, Selenastrum capricornutum (Slooff et al. 1983)
LC50 values to crustaceans, mg/l	5.4 4 1.9	48hr, Daphnia pulex (Canton & Adema 1978) 48hr, Asellus aquaticus (Slooff 1983) 48hr, Gammarus pulex (Slooff 1983)
LC50 values to fishes, mg/l	1.35	48hr, Salmo gairdneri (Slooff et al. 1983)
Other information about water organisms	LOEC 1.4 mg/l, rpd, schr, Entosiphon sulcatum (Bringmann & Kühn 1980a). LC50, 48hr, 1.8 mg/l, Tubificidae LC50, 48hr, 9.3 mg/l, Chironomus gr. thummi LC50, 48hr, 8.1 mg/l, Erpobdella octoculata LC50, 48hr, 6.5 mg/l, Lymnaea stagnalis LC50, 48hr, 6.6 mg/l, Dugesia cf. lugubris LC50, 48hr, 7.1 mg/l, Hydra oligactis LC50, 48hr, 13 mg/l, Corixa punctata LC50, 48hr, 12 mg/l, Ischura elegans LC50, 48hr, 1.3 mg/l, Nemoura cinerea LC50, 48hr, 13 mg/l, Cloeon dipterum (Slooff 1983) Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 4.9 mg/l protozoa (Entosiphon sulcatum): 1.4 mg/l (Bringmann & Kühn 1980a)	

ST

1751 • Salicylic acid

69-72-7

Sumformula of the chemical	C7H6O3	
EINECS-number	2007123	
Boiling point, °C	211	20 mmHg (MITI 1992)

Total degradation in water	Biodegradation: 88.1% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

1752 • SD 3450

14458-95-8

Other information about mammals	ALD = 5.5 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987).	
LD50 values to birds in oral exposure, mg/kg	< 25	orl-Agelaius phoeniceus (Schafer et al. 1983)

1753 • Selenium and selenium compounds

7782-49-2

LC50 values to crustaceans, mg/l	0.43	48hr, Daphnia magna (LeBlanc 1980)
	3.87	48hr, Daphnia magna (Reading & Buikema 1983)
LC50 values to fishes, mg/l	6.7	96hr, Cyprinodon variegarus (Heitmuller et al. 1981)
	1.325 2.4 1.55	sfd, 96hr, Morone saxatilis hrd, 96hr, Morone saxatilis 1%., 96hr, Morone saxatilis (Palawski et al. 1985)
	7.4	96hr, Cyprinodon variegarus (Ward et al. 1981)
	1	96hr, Pimephales promelas (Halter et al. 1980)
	5.17	Se(VI)28d, Salmo gairdneri (Birge et al. 1980)

1754 • Selenium dioxide

7446-08-4

LC50 values to fishes, mg/l	12	7d, Carassius auratus (Kemp et al. 1973)

1755 • Siduron

1982-49-6

Use	Herbicide.
Effects on plants	Severe thinning of bermudagrass occurred with siduron at 13 kg ai/ha (Callahan 1980).

1756 • Silicic acid, disodium salt

6834-92-0

Synonyms	Disodium metasilicate Disodium monosilicate Sodiummetasilicate Sodium silicate Water glass
Sumformula of the chemical	O3Si.2Na
Molecular weight	122.07

ST

LD50 values to mammals in oral exposure, mg/kg	770 1153	orl-mus orl-rat (Sweet 1987)
LDLo values to mammals in oral exposure, mg/kg	250 250	orl-dog orl-pig (Sweet 1987)
LDLo values to mammals in non-oral exposure, mg/kg	200	ipr-gpg (Sweet 1987)
TDLo values to mammals in oral exposure, mg/kg	15000	orl-rat, effects on newborn (Sweet 1987)
TDLo values to mammals in non-oral exposure, mg/kg	9.766 9.766	intratesticular-rat, paternal effects scu-rat, paternal effects (Sweet 1987)
Other information about mammals	Skin and eye irritation data; skin, human, 250 mg, 24hr, severe; skin, rabbit, 250 mg, 24hr, severe; skin, guinea pig, 250 mg, 24hr, moderate (Sweet 1987).	
LD50 values to birds in oral exposure, mg/kg	> 100	orl-Agelaius phoeniceus (Schafer et al. 1983)

1757 • Silver chloride 7783-90-6

Sumformula of the chemical	AgCl	
Use	Photography, photometry and optixs, batteries, photochromic glass, silver plating, production of pure silver, antiseptic. Single crystals are used for infrared absorption cells and lens elements, lab reagent.	
State and appearance	White, granular powder which darkens on exposure to light, finally turning black; exists in several modifications differing in behavior toward light and in their solubility in various solvents.	
Water solubility, mg/l	1.9	25 °C
Effects on the physiology of water organisms	Nostoc muscorum, 0.004 mg/l, 0.02 d, photosynthesis effect (Rai & Raizada 1987).	

1758 • Silver compounds 7440-22-4

Sumformula of the chemical	Ag
Use	Manufacture of silver nitrate, silver bromide, photographic chemicals; lining vats and other equipment for chemical reaction vessels, water distillation, etc.; mirrors, electric conductors, such as bus bars; silver plating, electronic equipments; sterilant; water purification; surgical cements; hydration and oxidation catalyst; special batteries, solar cells; reflectors for solar towers; low temperature brazing alloys; table cutlery; jewelry; dental, medical, and scientific equipment; electrical contacts; bearing metal; magnet windings; dental amalgams. Colloidal silver is used as a nucleating agent in photography and in medicine, often combined with protein.
State and appearance	Soft, ductile, lustrous, white solid; highest electrical and thermal conductivity of all metal. Excellent light reflector that resists oxidation, but tarnishes in air through reaction with atmospheric compounds.
Molecular weight	107.87
Melting point, °C	961
Boiling point, °C	2212

Mobility	Ag can appear in ion form (Ag+, Ag2+), as AgCl, as chloride complexes and as anion complexes (AgO-, Ag(S2O3)23-, Ag(SO)423-) in the environment (Kabata-Pendias & Pendias 1984). In soil mobile silver complexes become immobile around pH 4 (Kabata-Pendias & Pendias 1984). Ag is absorbed and bound to complexes with humus both in soil and water environments (Kabata-Pendias & Pendias 1984). Soluble in nitric acid, hot sulfuric acid, and alkali cyanide solutions; insoluble in water and alkalies. Noncombustible except as powder.
Metabolism in mammals	Silver is absorbed both via lungs and in alimentary canal (Tipton & Cook 1963). Excreting of silver is 8 times greater via faeces than via urine (Tipton et al. 1966).
Bioconcentration factor, fishes	< 1 28d, Lepomis (USEPA 1980)
Bioconcentration factor, mollusca	0.03-8 tissue/sediment (Luoma & Jenne 1977)
Bioconcentration factor, algae	210 calc., plankton 240 calc., brown algae (Bowen 1966) 620-15000 phytoplankton (Cushing & Rancitelli 1972)
LD50 values to mammals in oral exposure, mg/kg	100 orl-mus, colloidal Ag (Christensen 1973)
Health effects	An experimental tumorigen. Human systemic effects by inhalation: skin effects. Inhalation of dusts can cause argyrosis.
Carcinogenicity	Intravenous injektion of colloidal Ag induces tumors in rats (Furst & Haro 1969). Ag is not considered carcinogen (USEPA 1980).
Teratogenicity	No teratogenic effects have been observed in chicken embryos (4 than 8 days old) (Ridgeway & Karnofsky 1952).
Effects on amphibia	LD50 (96hr), 0.026 mg/l, tadpoles of Rana hexadactyla (Khangarot et al. 1985).
LC50 values to crustaceans, mg/l	0.0006–0.0550 Ag+,48hr, Daphnia magna (Barera & Adams 1983) 0.0015 48hr, Daphnia magna (LeBlanc 1980)
EC50 values to crustaceans, mg/l	0.01 48hr, mbt, Daphnia magna (Khangarot & Ray 1987)
LC50 values to fishes, mg/l	0.1 72hr, Cyprinus carpio 0.047 72hr, Carassius auratus (Ding et al.1982) 0.029 96hr, Salmo gairdneri (Khangarot & Ray 1987)
LOEC values to fishes, mg/l	0.0001 Salmo gairdneri (Nebeker et al.1983a) 0.00017 srv, schr, Salmo gairdneri (Davies et al. 1978)
NOEC values to fishes, mg/l	0.0001 grw, schr, Salmo gairdneri (Davies et al. 1978)
Other information	Source: Chief silver ores are native silver, argentite (silver sulfide), and cerargyrite (silver cloride).

1759 • Silver nitrate

7761-88-8

Sumformula of the chemical	AgNO3
Use	Photographic film, catalyst for ethylene oxide, indelible inks, silver plating, silver salts, silvering mirrors, germicide (as a wall spray), hair dyeing, antiseptic, fused form to cauterize wounds, lab reagent.

ST

State and appearance	Colourless, transparent, tabular, rhombic crystals becoming gray or grayish-black on exposure to light in the presence of organic matter.	
Odour	Odourless; bitter, caustic metallic taste.	
Molecular weight	169.88	
Water solubility, mg/l	2160000	25 °C
Melting point, °C	212	
Degradation point, °C	444	
LD50 values to mammals in oral exposure, mg/kg	50	orl-mus (Lewis & Sweet 1984)
	129	orl-mus (Christensen 1973)
LD50 values to mammals in non-oral exposure, mg/kg	34.5	ipr-mus (Sax & Lewis 1989)
LDLo values to mammals in oral exposure, mg/kg	20	orl-dog (Lewis & Sweet 1984)
	800	orl-rbt (Sax & Lewis 1989)
LDLo values to mammals in non-oral exposure, mg/kg	8.8 216 62	ivn-rbt ipr-gpg scu-gpg (Sax & Lewis 1989)
TDLo values to mammals in non-oral exposure, mg/kg	13.59 50 15000	scu-rat scu-dog skn-mus (Sax & Lewis 1989)
Health effects	Human poison by an unspecified route. Experimental poison by ingestion, intravenous, subcutaneous and intraperitoneal routes. An experimental tumorigen. Experimental reproductive effects. Human mutagenic data. A severe eye irritant. A powerful caustic and irritant to skin, eyes and mucous membranes. Swallowing can cause severe gastroenteritis that may be fatal.	
Effects on arthropods	Tanytarsus dissimilis, LC50, 2 d, 0.420 mg/l (Holcombe et al. 1987).	
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 0.006 mg/l (Bringmann & Kühn 1980a)	
EC50 values to algae, mg/l	0.17	96hr, Skeletonema costatum, pht (USEPA 1980)
LOEC values to algae, mg/l	0.05	Scenedesmus (Bringmann & Kühn 1959)
LC50 values to crustaceans, mg/l	0.042 0.015	1d, Daphnia magna 2d, Daphnia magna (Khangarot et al. 1987)
	0.56	4d, Orconectes immunis (Holcombe et al. 1987)
EC50 values to crustaceans, mg/l	0.006 0.005	2d, mbt, Crangonyx pseudogracilis 4d, mbt, Crangonyx pseudogracilis (Martin & Holdich 1986)
	0.023 0.01	1d, mbt, Daphnia magna 2d, mbt, Daphnia magna (Khangarot & Ray 1987)
	0.0009	2d, mbt, Daphnia magna (Holcombe et al. 1987)

ST

LC50 values to fishes, mg/l	0.029	96hr, Salmo gairdneri (Hale 1977)
	0.0067	96hr, flow-through, Pimephales promelas
	0.014	96hr, static, Pimephales promelas
	0.0173	96hr, flow-through, Ictalurus punctatus (Holcombe et al. 1983)
	0.06	96hr, Lepomis macrochirus (Buccafusco et al. 1981)
	0.013	4d, Lepomis macrochirus
	0.009	4d, Pimephales promelas
	0.006	4d, Salmo gairdneri (Holcombe et al. 1987)
LOEC values to fishes, mg/l	0.0001	Salmo gairdneri (Nebeker et al. 1983)
Other information about water organisms	Aplexa hypnorum, LC50, 4 d, 0.083 mg/l (Holcombe et al. 1987). LC50, 0.241 mg/l, 96hr, renewal, Aplexa hypnorum (Holcombe et al. 1983) Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 0.0095 mg/l protozoa (Entosiphon sulcatum): 0.58 mg/l (Bringmann & Kühn 1980a) Chlorella vulgaris, effects on growth, 0.03 mg/l (Stokes 1973). Chlorella fusca, EC100, 0.1 mg/l (Stokes 1973). Gastropoda, LC50, 96hr, 0.241 mg/l (Holcombe et al. 1983). Crassostrea virginica, larvae, LC50, 48hr, 0.0046–0.0064 mg/l (Calabrese et al. 1973). Salmo gairdneri, eggs, juv., LC100, 0,0013 mg/l (Nebeker et al. 1983). Salvelinus fontinalis, MATC, 0.00009–0.00017 mg/l (Davies 1975).	

1760 • Silver sulfide

21548-73-2

Sumformula of the chemical	Ag2S
Use	Inlaying in niello metal-work, ceramics.
State and appearance	Grayish black powder, soluble in concentrated sulfuric and nitric acids, insoluble in water.
Melting point, °C	825

1761 • Simazine

122-34-9

Synonyms	2-Chloro-4,6-bis(ethylamino)-s-triazine Princep	
Use	Active ingredient in herbicides.	
Molecular weight	201.69	
Water solubility, mg/l	5	20 °C
	3.5	(MITI 1992)
Melting point, °C	225–227	(MITI 1992)
Log soil sorption coefficient, log Kom	2.13	(Sabljic 1987)
Half-life in soil, days	75	(Li et al. 1990)
Total degradation in soil	75–100% disappearance from soils: 12 months (Verschueren 1983).	

ST

Total degradation in water	Biodegradation: 0.7% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	2.3–3.2 9.7–14.6	6w, Cyprinus carpio, conc 0.1 mg/l 6w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
LD50 values to mammals in oral exposure, mg/kg	5000	orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	1400	unk-mam (Lewis & Sweet 1984)
Other information about mammals	In diet: rat, 100 ppm for 2 years: nontoxic (Martin 1968).	
Effects on plants	The phytotoxic limiting concentration 0.01 mg simazine/kg soil. (Ladonin & Lunev 1983) Seeds of Senecio vulgaris were sown onto the surface of compost containing 0.7 kg simazine/ha a.i. → mean percentage mortality of plants 16 weeks after sowing was > 90%. (Holiday & Putwain 1977)	
EC50 values to algae, mg/l	0.5	rpd, Isochrysis galbana (Walsh 1972) Phaeodactylum tricornurum
LC50 values to crustaceans, mg/l	3.2 13 1 > 40 1	48hr, Cypridopsis vidua 96hr, Gammarus lacustris 48hr, Daphnia magna (Sanders 1970) act, Daphnia pulex (Hashimoto & Nishiuchi 1981) act, Daphnia magna (Kenaga 1979)
NOEC values to crustaceans, mg/l	100	48hr, Gammarus fasciatus Asellus brevicaudus Palaemonetes kadiakensis Orconectes nais (Sanders 1970)
LC50 values to fishes, mg/l	12.6 3.1 24.5 25 6.6 > 100 90 > 40 > 40 > 10	96hr, Branchydanio rerio 96hr, Sarotherodon aureus 96hr, Barbus ticto ticto (Verschueren 1983) Salmo gairdneri (Kenaga 1979) 48hr, Oncorhynchus kisutch (Bond et al. 1960) 96hr, Salmo gairdneri 96hr, Lepomis macrochirus (Pesticide Manual 1983) 48hr, Carassius auratus 48hr, Cyprinus carpio (Hashimoto & Nishiuchi 1981) 48hr, Oryzias latipes (MITI 1992)

Effects on the physiology of water organisms	Algae: Chlorococcum sp. (technical acid): 2500 ppb: 50% decrease in 02 evolution; 2000 ppb: 50% decrease in growth (measured as ABS (525 mu) after 10 days) Dunaliella tertiolecta (technical acid): 4000 ppb: 50% decrease in 02 evolution; 5000 ppb: 50% decrease in growth (measured as ABS (525 mu) after 10 days) Isochrysis galbana (technical acid): 600 ppb: 50% decrease in 02 evolution; 500 ppb: 50% decrease in growth (measured as ABS (525 mu) after 10 days) Phaeodactylum tricornutum (technical acid): 600 ppb: 50% decrease in 02 evolution; 500 ppb: 50% decrease in growth (measured as ABS (525 mu) after 10 days) (Walsh 1972).

1762 • Slimacide V10 * 20679-58-7

Synonyms	Bis(1,4-bromoacetoxy)-2-butene	
Active ingredients	Bis-1,4-bromoacetoxy-2-butene	
Use	Slimicide.	
Total degradation in water	Biodegradation: 33–74% by BOD (on the upward trend) period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LC50 values to crustaceans, mg/l	5	48hr, Asellus (Landner et al.1973)
	0.24	96hr, 21 °C, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	1 2.1	24hr, Rasbora heteromorpha 24hr, Poecilia reticulata (Landner et al. 1973)
	0.52	96hr, 10 °C, Alburnus alburnus (Linden et al. 1979)
Other information about water organisms	LC50 (72hr), 8.0 mg/l, Anodonta cygnea (Landner et al. 1973).	

1763 • Sodium 3-nitrobenzene sulfonate 127-68-4

Synonyms	Sodium m-nitrobenzenesulfonate m-Nitrobenzenesulfonic acid, sodium salt
Sumformula of the chemical	C6H4NO5S.Na
Molecular weight	225.16

ST

Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.5–1.6 6w, Cyprinus carpio, conc 1 mg/l < 5 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	11000 orl-rat (Sweet 1987)
Other information about mammals	Skin and eye irritation data: skin, rabbit, 500 mg, 24hr, mild; eye, rabbit, 20 mg, 24hr, moderate (Sweet 1987).
LC50 values to crustaceans, mg/l	5100 96hr, Daphnia magna (Dowden & Bennet 1965)
LC50 values to fishes, mg/l	> 1000 48hr, Oryzias latipes (MITI 1992)

1764 • Sodium 4,4'-diamino-2,2'-stilbene disulfonate 25394-13-2

Water solubility, mg/l	> 2000 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.2 6w, Cyprinus carpio, conc 2 mg/l < 1.9 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 200 48hr, Oryzias latipes (MITI 1992)

1765 • Sodium 4-nitrochlorobenzene sulfonate 946-30-5

Sumformula of the chemical	C6H3O5NSClNa
Total degradation in water	Biodegradaation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.3 6w, Cyprinus carpio, conc 3 mg/l < 3.0 6w, Cyprinus carpio, conc 0.3 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 1000 48hr, Oryzias latipes (MITI 1992)

ST

1766 • Sodium acetate

129-09-3

LC50 values to fishes, mg/l	5	24hr, Lepomis macrochirus (Dowden 1960)

1767 • Sodium alloxidine

55634-91-8 (alloxydim)
66003-55-2 (sodium alloxydim)

Use	Herbicide.	
LC50 values to fishes, mg/l	3500	48hr, Cyprinus carpio (Pesticide Manual 1983)

1768 • Sodium and sodium compounds

7440-23-5

LC50 values to crustaceans, mg/l	1480 1640 1820	21d, Daphnia magna 48hr, without food, D.magna 48hr, with food, D.magna (Biesinger & Christensen 1972)
EC50 values to crustaceans, mg/l	1020	21d, rpd, Daphnia magna (Biesinger & Christensen 1972)
LOEC values to crustaceans, mg/l	680	21d, rpd, schr, Daphnia magna (Biesinger & Christensen 1972)

1769 • Sodium benzenesulfinic acid

618-41-7

Sumformula of the chemical	C6H5O2SNa
Melting point, °C	83–84 (MITI 1992)
Total degradation in water	Biodegradation: 99% by BOD period: 21d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).

1770 • Sodium bicarbonate

144-55-8

LC50 values to fishes, mg/l	8600	96hr, Lepomis macrochirus (Kemp et al. 1973)

1771 • Sodium bromide

7647-15-6

Sumformula of the chemical	NaBr	
Molecular weight	79.9	
LD50 values to mammals in oral exposure, mg/kg	3500	orl-rat (Lewis & Sweet 1984)
Effects on amphibia	NOEC, 32 mg/l, 100d, Xenopus laevis, mortality NOEC, 320 mg/l, 100d, Xenopus laevis, development NOEC, 320 mg/l, 100d, Xenopus laevis, growth (Slooff & Canton 1983)	

ST

Effects on arthropods	NOEC, 100 mg/l, 25d, Culex pipiens, mortality NOEC, 100 mg/l, 25d, Culex pipiens, development (Slooff & Canton 1983)
Effects on plants	NOEC, 3200 mg/l, 7d, Lemna minor, specific growth rate. (Slooff & Canton 1983)
Effects on microorganisms	NOEC, 3200 mg/l, 0.3d, Pseudomonas fluorescens, specific growth rate. NOEC, 3200 mg/l, 4d, Microcystis aeruginosa, specific growth rate. (Slooff & Canton 1983) Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 2175 mg/l (Bringmann & Kühn 1980a)
EC50 values to algae, mg/l	0.008 rpd, act, 48hr, green algae (Canton et al. 1983)
NOEC values to algae, mg/l	3200 4d, grw (biomass), Scenedesmus pannonicus (Slooff & Canton 1983)
LC50 values to crustaceans, mg/l	0.011 48hr, Daphnia magna (Canton et al. 1983) 1 48hr, Daphnia magna (LeBlanc 1980) 13500 48hr, Daphnia magna (Hermens et al. 1984)
EC50 values to crustaceans, mg/l	29 16d, rpd, Daphnia magna (Hermens et al. 1984)
NOEC values to crustaceans, mg/l	3200 21d, srv, Daphnia magna 10 21d, rpd, Daphnia magna (Slooff & Canton 1983)
LC50 values to fishes, mg/l	0.016 96hr, Poecilia reticulata (Canton et al. 1983)
EC50 values to fishes, mg/l	180–225 125d, srv, Poecilia reticulata (Hermens et al. 1984)
NOEC values to fishes, mg/l	100 28d, srv, Poecilia reticulata 32 28d, srv + bhv, Poecilia reticulata 320 28d, grw, Poecilia reticulata 3200 40d, srv, Oryzias latipes 320 40d, srv + bhv, Oryzias latipes 10000 40d, grw, Oryzias latipes (Slooff & Canton 1983)
Other information about water organisms	NOEC, 1000 mg/l, 21d, Hydra oligactis, specific growth rate. NOEC, 3200 mg/l, 40d, Lymnaea stagnalis, mortality. NOEC, 10 mg/l, 40d, Lymnaea stagnalis, reproduction. NOEC, 3200 mg/l, 40d, Lymnaea stagnalis, hatching. (Slooff & Canton 1983) Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 2800 mg/l protozoa (Entosiphon sulcatum): 116 mg/l (Bringmann & Kühn 1980a)

1772 • Sodium carbonate 497-19-8

Synonyms	Carbonic acid, disodium salt Crystolcarbonate Soda ash
Sumformula of the chemical	CO3.2Na
Molecular weight	105.99
LD50 values to mammals in oral exposure, mg/kg	4090 orl-rat (Sweet 1987)

ST

LD50 values to mammals in non-oral exposure, mg/kg	117 2210	ipr-mus scu-mus (Sweet 1987)
LC50 values to mammals in inhalation exposure, mg/m³	800 1200 2300	ihl-gpg ihl-mus ihl-rat (Sweet 1987)
Other information about mammals	Skin and eye irritation: skin, rabbit, 500 mg, 24hr, mild; eye, rabbit, 100 mg, 24hr, moderate; eye, rabbit, 100 mg rinse, mild (Sweet 1987).	

1773 • Sodium chloride

7647-14-5

LC50 values to fishes, mg/l	17.9	96hr, Anguilla rostrata (Hinton & Eversole 1978)
	13000.9	96hr, Lepomis macrochirus (Kemp et al. 1973)

1774 • Sodium cyanide

143-33-9

Sumformula of the chemical	NaCN	
Use	Extraction of gold and silver from ores, elctroplating, heat treatment of metals (case-hardening), making hydrogen cyanide, insecticide, cleaning metals, fumigation, manufacture of dyes and pigments, nylon intermediates, chelating compounds, ore flotation.	
State and appearance	White deliquescent, crystalline powder; soluble in water; slighly soluble in alcohol.	
Molecular weight	49.01	
Vapour pressure, mmHg	1	817 °C
Melting point, °C	563	
Boiling point, °C	1496	
Other physicochemical properties	The aqueous solution is strongly alkaline and decomposes rapidly on standing.	
LD50 values to mammals in oral exposure, mg/kg	6.44 4	orl-rat orl-dom (Sax & Lewis 1989)
LD50 values to mammals in non-oral exposure, mg/kg	4.3 5.881 3.66 1.666 5.8	ipr-rat ipr-mus scu-mus ims-rbt scu-gpg (Sax & Lewis 1989)
LDLo values to mammals in oral exposure, mg/kg	6.557 2.857	orl-man orl-hmn (Sax & Lewis 1989)
LDLo values to mammals in non-oral exposure, mg/kg	6 1.3 2.2	scu-dog ivn-dog scu-rbt (Sax & Lewis 1989)

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TDLo values to mammals in oral exposure, mg/kg	0.714 orl-man (Sax & Lewis 1989)
TDLo values to mammals in non-oral exposure, mg/kg	5999 imp-ham, 6-9d preg, teratogenic effect 5928 imp-ham, 6-9d preg, teratogenic effect (Sax & Lewis 1989)
Health effects	Toxic by ingestion and inhalation (Sax & Lewis 1987).
Effects on the physiology of water organisms	Salmo gairdneri, physiological effect, 2 days, 0.0005 mM (Dixon et al. 1987).

1775 • Sodium deoxycholate 302-95-4

Other information about water organisms	Poteriochromonas malhamensis, 37.4 mg/l, 3 d, 100% mortality (Roderer 1987).

1776 • Sodium dichromate 10588-01-9

Synonyms	Sodium bichromate Chromic acid, disodium salt
Sumformula of the chemical	Na2Cr2O7
Use	Colourimeter (Copper determination), complexing agent, oxidation inhibitor in ethyl ether.
State and appearance	Red or red-orange deliquescent crystals.
Melting point, °C	357
Degradation point, °C	400
Other physicochemical properties	Soluble in water, insoluble in alcohol. Noncombustible.
LD50 values to mammals in oral exposure, mg/kg	50 orl-rat (Sax & Lewis 1989)
LDLo values to mammals in non-oral exposure, mg/kg	80 scu-rat 26.2 ivn-mus 18.4 ivn-rbt 335 ipr-gpg 23 scu-gpg (Sax & Lewis 1989)
Health effects	A toxic material (Sax & Lewis 1987). Poison by ingestion, skin contact, intravenous, intraperitoneal, and subcutaneous routes. An experimental tumorigen. Chromate salts are considered to be carcinogens. Human mutagenic data. A caustic and irritant (Sax & Lewis 1989).
Mutagenicity	mma, sat, 0.030 mg/plate; cyt, hmn, lym, 0.002 mmol/l; dnd, rat, lvr, 3 mmol/l; sce, ham, lng, 0.035 mg/l (Sax & Lewis 1989).
Effects on amphibia	LDLo, ivn-frg, 196 mg/kg (Sax & Lewis 1989).
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 0.78 mg/l (Bringmann & Kühn 1980a).
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 1.2 mg/l protozoa (Entosiphon sulcatum): 20 mg/l (Bringmann & Kühn 1980a).

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1777 • Sodium diisopropyl naphthalene sulfonate 1322-93-6

Total degradation in water	Biodegradation: 0% by BOD period: 14 d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.6–1.5 6w, Cyprinus crpio, conc 0.74 mg/l 2.9–5.1 6w, Cyprinus carpio, conc 0.074 mg/l, (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	275 48hr, Oryzias latipes (MITI 1992)

1778 • Sodium dinaphthyl methane disulfonate 26545-58-4

Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.6–1.2 6w, Cyprinus carpio, conc 2 mg/l < 1.0 6w, Cyprinus carpio, conc 2 mg/l < 0.3 6w, Cyprinus carpio, conc 2 mg/l < 0.1 6w, Cyprinus carpio, conc 2 mg/l < 6.6 6w, Cyprinus carpio, conc 0.2 mg/l < 10 6w, Cyprinus carpio, conc 0.2 mg/l < 2.5 6w, Cyprinus carpio, conc 0.2 mg/l < 1.4 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
LC50 values to fishes, mg/l	1019 48hr, Oryzias latipes (MITI 1992)

1779 • Sodium dodecylbenzene sulfonate 25155-30-0

Effects on the physiology of water organisms	Biochemical effect (change in physiochemical process including glycogen uptake, cholesterol levels and lipid analysis): Carassius carassius, 7.0 mg/l, 0.21d (Nakanishi et al. 1986b); Gnathopogon caerulescens; 0.1 mg/l, 1d (Nakanishi et al. 1987).
Other information about water organisms	Carassius carassius, 7.0 mg/l, 100% mortality (Nakanishi et al. 1986b).

1780 • Sodium fluoride 7681-49-4

Sumformula of the chemical	NaF
Use	NF is used mostly as an additive e.g. in tooth pastes and medicines.
Water solubility, mg/l	42000 10 °C

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Melting point, °C	992	
Boiling point, °C	1704	
LD50 values to mammals in non-oral exposure, mg/kg	10	24hr, ipr-small rodents (Hodge & Smith 1965)
Other information about mammals	Tolerance limit for chronic injuries in mammals: cattle, annual average: 30–50 mg/kg dry weight as NaF in food (Eagers 1969).	
LD50 values to birds in oral exposure, mg/kg	> 200	orl-Sturnus vulgaris (Schafer et al. 1983)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 231 mg/l (Bringmann & Kühn 1980a)	
LC50 values to algae, mg/l	43	96hr, rpd, Scenedesmus (McKee & Wolf 1963)
LC50 values to crustaceans, mg/l	340	48hr, Daphnia magna (LeBlanc 1980)
	300	NaF, 48hr, shrimp (Sax 1986)
EC50 values to crustaceans, mg/l	98	F-, 48hr, Daphnia (Dave 1984)
Effects on the physiology of water organisms	Indonaia caerulea, biochemical, oxygen consumption and other physiological effects, 0.04–0.50 days, 0.5 mg/l (Mane et al. 1987).	
Other information about water organisms	4.5 mg/l NaF, lobster, not toxic; 7.2 mg/l NaF, 108hr, brown mussels, toxic effect; 52 mg/l, 72 d, mullet, crab, physical deterioration; 52 mg/l NaF, 72 d, shrimp, affects reproduction (Sax 1986). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 249 mg/l protozoa (Entosiphon sulcatum): 101 mg/l (Bringmann & Kühn 1980a).	

1781 • Sodium fluoroacetate 62-74-8

Other information about mammals	ALD = 3.7–5.5 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987).

1782 • Sodium formaldehyde sulfoxylate 149-44-0

Synonyms	Methanesulfinic acid, hydroxy-, monosodium salt	
Sumformula of the chemical	CH4O3S.Na	
EINECS-number	2057394	
Water solubility, mg/l	> 100000	(MITI 1992)
Melting point, °C	63–64	(MITI 1992)
Total degradation in water	Biodegradation: 89–116% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

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1783 • Sodium hydroxide

1310-73-2

Synonyms	NAOH Caustic soda Sodium hydrate Soda lye
Sumformula of the chemical	HNaO
Use	Cellulose; rubber manufacturing; intermediate; medicine; rayon manufacturing; veterinary.
State and appearance	White deliquescent solid or solution. Will dissolve.
Molecular weight	40
Specific gravity (water=1)	2.13
Vapour pressure, mmHg	100 1111 °C
Water solubility, mg/l	480000 25 °C
Melting point, °C	318
Boiling point, °C	1390
Other information about degradation	Can persist for extended periods of time (Sax 1986).
Other information about bioaccumulation	Potential for accumulation: negative (Sax 1986).
LD50 values to mammals in non-oral exposure, mg/kg	40 ipr-mus (Sax 1986)
LDLo values to mammals in oral exposure, mg/kg	500 orl-rbt (Sax 1986)
Other information about mammals	Skin and eye irritation data: eye, monkey, 1%, 24hr, severe; skin, rabbit, 500 mg, 24hr, severe; eye, rabbit 0.4 mg, mild; eye, rabbit, 1%, severe; eye, rabbit, 0.050 mg, 24hr, severe; eye, rabbit, 1 mg, 24hr, severe; eye, rabbit, 100 mg rinse, severe (Sweet 1987).
Health effects	Direct contact: Causes burns and deep ulceration, can destroy tissue (Sax 1986). Inhalation of dust may seriously affect lungs. Ingestion causes severe tissue damage (Sax 1986).
Mutagenicity	cyt-grh-par 20 mg (Sax 1986).
Effects on wastewater treatment	Can raise pH and interfere with coagulation (Sax 1986).
LC50 values to crustaceans, mg/l	33–100 48hr, Crangon crangon (Kemp et al. 1973)
LC50 values to fishes, mg/l	33–100 48hr, salt water starfish (Sax 1986)
Other information about water organisms	100 mg/l, Daphnia, minnows, lethal; 40–240 mg/l, Daphnia magna, toxicity threshold; 125–1000 mg/l, various insect larvae, lethal; 25 mg/l, 24hr, brook trout, lethal; 70 mg/l, 5hr, fish, crabs, lethal; 90 mg/l, 4.5hr, oysters, lethal, salt water; 180 mg/l, 23hr, oysters, lethal, salt water (Sax 1986).

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Other information	The toxicity of sodium hydroxide is based on the increasing pH-value it induces. Thus the toxic dose is dependent on the buffer capacity of the dilution water. Forms corrosive alkaline solution. Will precipitate many cations present in water (Sax 1986). Taste threshold: lower 1 ppm, upper 50 ppm (Sax 1986). High sodium levels can disperse soils (Sax 1986).

1784 • Sodium hypochlorite 7681-52-9

Molecular weight	75.45	
Effects on plants	Seed tubers of potatoes for main-crop planting of 'Rua' and 'Whitu' yielded about 10% less after dipping in a 1% solution of sodium hypochlorite for longer than 1 h. After 4 months storage field emergence of 'Rua' was significantly reduced. (Bedi & Genet 1977)	
LC50 values to crustaceans, mg/l	40	96hr, 10 °C, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	0.07	(C12), 48hr, Salmo gairdneri (Nikunen et al. 1985)
	5.9	96hr, Pimephales promelas (Curtis et al. 1979)
	32–37	96hr, 10 °C, Alburnus alburnus (Linden et al. 1979)
LOEC values to fishes, mg/l	0.02	C12, srv, schr, Oncorhynchus kisutch (Larson et al. 1978)
Effects on the reproduction of water organisms	Piscicola salmotica, 0.094 mg/l, 1 d, change in percent hatch or time to hatch (Bower & Thompson 1987).	

1785 • Sodium(I) nitrate 7631-99-4

Synonyms	Nitric acid, sodium salt	
Sumformula of the chemical	NO3.Na	
Molecular weight	85	
LD50 values to mammals in oral exposure, mg/kg	3236	orl-rat
	2680	orl-rbt (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	175	ivn-mus (Sweet 1987)
LDLo values to mammals in oral exposure, mg/kg	114	orl-man (Sweet 1987)
TDLo values to mammals in oral exposure, mg/kg	100000	orl-rat, tumorigenic (Sweet 1987)
Mutagenicity	Mutation data: cytogenetic analysis: ham, fbr, 7200 mg/l, 48hr; ham, lug, 5700 mg/l; mus, orl. 7067 mg/kg; rat, orl. 78.5 mg/kg; host-mediated assay: ham, emb, 125 mg/kg; micronucleus test: ham, orl, 250 mg/kg; mus, orl, 78.5 mg/kg; microbial mutation without S9: microorganisms, 1000 ppm;	

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	oncogenic transformation: ham, orl, 250 mg/kg (Sweet 1987).

1786 • Sodium lauryl sulfate 151-21-3

Use	Wetting agent in textiles; detergent in toothpaste; food additive and surfactant.
State and appearance	Small white and yellow crystals.
Molecular weight	289.43
Melting point, °C	204–207
Total degradation in water	Biodegradation: 85% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Other information about degradation	Biodegradation (17 mg/l): no degradation after 30 days (Verschueren 1983).
LD50 values to mammals in oral exposure, mg/kg	1288 orl-rat (Lewis & Sweet 1984)
LOEC values to algae, mg/l	0.02 rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
LC50 values to fishes, mg/l	8.1 96hr, Jordanella floridae 8 96hr, Brachydanio rerio 4.6 96hr, Salmo trutta (Fogels & Sprague 1977)
Other information about water organisms	LOEC 0.75 mg/l, rpd, schr, Uronema parduczi (Bringmann & Kühn 1980b). Poteriochromonas malhamensis, 89.3 mg/l, 3 d, 100% mortality including algicidal and herbicidal effects (Roderer 1987).

1787 • Sodium lauryl sulfonate 2386-53-0

Effects on the physiology of water organisms	Cyprinus carpio, 6.1 mg/l, 0.17 d, biochemical effect (change in physiochemical process including glycogen uptake, cholesterol levels and lipid analysis) (Nakanishi et al. 1986a).

1788 • Sodium molybdate 7631-95-0

EC50 values to crustaceans, mg/l	3618 2d, mbt, Crangonyx pseudogracilis 2650 4d, mbt, Crangonyx pseudogracilis (Martin & Holdich 1986)

1789 • Sodium naphthenate 61790-13-4

Water solubility, mg/l	> 100000 (MITI 1992)
Melting point, °C	125–146 (MITI 1992)

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Total degradation in water	Biodegradation: 33–58% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).	
Bioconcentration factor, fishes	1.6–4.4 < 10–13	6w, Cyprinus carpio, conc 0.5 mg/l 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
LC50 values to fishes, mg/l	260	48hr, Oryzias latipes (MITI 1992)

1790 • Sodium naphthionate 28907-84-8

Synonyms	2-Naphthalenesulfonic acid, 5-amino-, sodium salt
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).

1791 • Sodium nitrite 7632-00-0

Synonyms	Nitrous acid, sodium salt	
Sumformula of the chemical	NO2.Na	
Molecular weight	69	
LD50 values to mammals in oral exposure, mg/kg	175 85 186	orl-mus orl-rat orl-rbt (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	158 65	ipr-mus ivn-rat (Sweet 1987)
LDLo values to mammals in oral exposure, mg/kg	1500 22 330 71	orl-cat orl-child orl-dog orl-hmn (Sweet 1987)
LDLo values to mammals in non-oral exposure, mg/kg	15 80 35 60 150 10 60	ivn-dog ivn-rbt scu-cat scu-dog scu-mus scu-rat scu-rbt (Sweet 1987)

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TDLo values to mammals in oral exposure, mg/kg	280 orl-mus, 1-14d preg. specific developmental abnormalities 660 orl-rat, 1-22d preg. effects on embryo of fetus effects on newborn 11000 orl-rat, 1-22d preg. effects on newborn 40000 orl-rat, tumorigenic 14 orl-hmn, behavioral, gastrointestinal, vascular 1.714 orl-man, 70 min, cardiac, vascular (Sweet 1987)
Other information about mammals	Skin and eye irritation data: eye, rabbit, 500 mg, 24hr, mild (Sweet 1987).
Mutagenicity	Mutation data: body fluid assay: hmn, sat, 200 mmol/l; cyt, ham, fbr, 530 mg/l, 34hr; cyt, ham, lug, 400 mg/l; cyt, mus, mmr, 10 mmol/l, 24hr; cyt, rat, orl, 2730 mg/kg; dnd, mam, lym, 1 mol; dnd, microorganism, 1 mol/l; DNA inhibition: hmn, fbr, 2000 ppm; dns, hmn, hla, 6 mmol/l; mrc, smc, 0.1 mmol/l; gene mutation in mammalian cells: ham, lug, 1000 ppm; mnt, ham, orl, 500 mg/kg; microbial mutation without S9: bcs, 400 mol; microorganisms, 2 mol/l; microorganisms, 50 mmol/l; microorganisms, 700 mmol/l; sat, 0.250 mg/plate; ssp, 34 mmol/l; microsomal assay: sat, 9 mg/plate; otr, ham, orl, 100 mg/kg; sin, ham, fbr, 3 mmol/l (Sweet 1987).
Effects on amphibia	LDLo 1000 mg/kg, scu, frog (Sweet 1987).
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 123 mg/l (Bringmann & Kühn 1980a)
LC50 values to fishes, mg/l	200 96hr, Channa punctatus 64 96hr, Mystus vittatus 76.1 1d, Channa punctatus 40.6 4d, Channa punctatus 33.3 1d, Mystus vittatus 13 4d, Mystus vittatus (Ansari 1987a)
Effects on the physiology of water organisms	Semaprochilodus insignis, 0.04 d, 9.1 mg/l, hematological effect (change in various blood parameters such as red blood cell count, hematocrit, and serum osmolarity) (Bartlett et al. 1987).
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 1233 mg/l protozoa (Entosiphon sulcatum): 2.8 mg/l (Bringmann & Kühn 1980a).

1792 • Sodium oxalate 62-76-0

LC50 values to fishes, mg/l	630 96hr, Branchydanio rerio 160–325 48hr, Leuciscus idus (Wellens 1982)

1793 • Sodium pentachlorophenol 131-52-2

Effects on amphibia	LC50 (96hr), 0.018 mg/l, tadpoles of Rana hexadactyla (Khangarot et al. 1985).
LC50 values to fishes, mg/l	0.065 96hr, Oncorhynchus kisutch (Iwama & Greer 1980)
Effects on the physiology of water organisms	Oncorhynchus tshawytscha, 4 d, 0.0039 mg/l, hematological effect (change in various blood parameters such as red blood cell count, hematocrit, and serum osmolarity) (Iwama et al. 1986).

1794 • Sodium polyoxyethylene monoalkyl ether sulfate 9004-82-4

Sumformula of the chemical	(C2H4O)n.C12H26O4S.Na
Total degradation in water	Biodegradation: 59% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

1795 • Sodium propionate 137-40-6

LC50 values to fishes, mg/l	5000 96hr, Lepomis macrochirus (Dowden 1960)

1796 • Sodium salt of chloromethyl-sulfonamide tetrachlorodiphenylether derivatives 100468-92-6

Sumformula of the chemical	C13H12O3Cl5SNa
Water solubility, mg/l	< 10 (MITI 1992)
Total degradation in water	Biodegradation: 3% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	45–77 8w, Cyprinus carpio, conc 0.0005 mg/l 35–106 8w, Cyprinus carpio, conc 0.00005 mg/l (MITI 1992)
LC50 values to fishes, mg/l	0.22 48hr, Oryzias latipes (MITI 1992)

1797 • Sodium salts of phenolsulfonic acid 1300-51-2

Sumformula of the chemical	C6H5O4SNa
Water solubility, mg/l	> 200000 (MITI 1992)
Total degradation in water	Biodegradation: 86% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

1798 • Sodium selenate 13410-01-0

LC50 values to crustaceans, mg/l	1.51 0.58	1d, Daphnia magna 4d, Daphnia magna (Johnston 1987)

1799 • Sodium selenite 10102-18-8

Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 18 mg/l (Bringmann & Kühn 1980a).	
LC50 values to crustaceans, mg/l	1.65 0.44	1d, Daphnia magna 4d, Daphnia magna (Johnston 1987)
LC50 values to fishes, mg/l	8.1 1.8	96hr, Salmo gairdneri (Hodson et al. 1980) 4d, Salmo gairdneri (Hunn et al. 1987)
Effects on the physiology of water organisms	Salmo gairdneri, 0.1 mg/l, 30 d, change in length and/or weight (Baatrup & Danscher 1987).	
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 0.84 mg/l protozoa (Entosiphon sulcatum): 0.003 mg/l (Bringmann & Kühn 1980a).	

1800 • Sodium stearate 822-16-2

Effects on the physiology of water organisms	Cyprinus carpio, 6.0 mg/l, 0.17 d, biochemical effect (change in physiochemical process including glycogen uptake, cholesterol levels and lipid analysis) (Nakanishi et al 1986a).

1801 • Sodium sulfate 7757-82-6

Synonyms	Disodium sulfate Sulfuric acid disodium salt	
Sumformula of the chemical	O4S.2Na	
Molecular weight	142.04	
LD50 values to mammals in oral exposure, mg/kg	5989	orl-mus (Sweet 1987)
LDLo values to mammals in non-oral exposure, mg/kg	1220	ivn-mus (Sweet 1987)

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TDLo values to mammals in non-oral exposure, mg/kg	60	par-mus, 8d preg. effects on embryo or fetus specific developmental abnormalities (Sweet 1987)

1802 • Sodium sulfide 16721-80-5

Synonyms	Sodium mercaptan Sodium bisulfide Sodium hydrogen sulfide Sodium hydrosulfide Sodium sulfhydrate	
Sumformula of the chemical	HNaS	
Molecular weight	56.06	
LD50 values to mammals in non-oral exposure, mg/kg	30 18 200	ipr-rat (Lewis & Sweet 1984) ipr-mus scu-mus (Sweet 1987)
Mutagenicity	Mutation data: Microbial mutation without S9: sat, 2 µmol/plate; sex chromosome loss and nondisjunction: dmg, orl, 50 mmol/l (Sweet 1987).	
LC50 values to fishes, mg/l	0.7	120hr, Salmo clarci (Haudy et al. 1952)

1803 • Sodium=α-sulfonate-ω-nonylphenoxy polyoxyethylene (the polymerization grade 6) 9014-90-8

Sumformula of the chemical	(C2H4O)nC15H24O4S.Na	
Water solubility, mg/l	> 100000 (MITI 1992)	
Log octanol/water coefficient, log Pow	0.02	(MITI 1992)
Total degradation in water	Biodegradation: 21–46% by BOD substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 17–53 < 150	6w, Cyprinus carpio, conc 0.03 mg/l 6w, Cyprinus carpio, conc 0.003 mg/l (MITI 1992)
LC50 values to fishes, mg/l	3.36	48hr, Oryzias latipes (MITI 1992)

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1804 • Sodium trichloroacetate 650-51-1

Synonyms	TCA (Na-) Trichloroacetate (Na-)
Sumformula of the chemical	C2Cl3O2Na
Use	Active ingredient in herbicides.

Molecular weight	185.36
LD50 values to mammals in oral exposure, mg/kg	3320 orl-rat 3600 orl-mus (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	2370 ivn-mus 3000 unk-mam (Lewis & Sweet 1984)
LC50 values to crustaceans, mg/l	3100 96hr, Daphnia magna (Knapek & Lekola 1974) 1428 act, Daphnia magna (Kenaga 1979) 2000 48hr, Daphnia magna (Dennis et al. 1979)
LC50 values to fishes, mg/l	2500 96hr, Cyprinus carpio (Knapek & Lekola 1974) > 100 act, Salmo gairdneri (Kenaga 1979) 2000 96hr, Phoxinus phoxinus (Dennis et al. 1979)
Other information about water organisms	LC50 (96hr) 5500 mg/l, mosquito (Knapek & Lekola 1974).

1805 • Sodium vanadate 13718-26-8

LC50 values to crustaceans, mg/l	3.4–4.8 2d, Daphnia magna (Beusen & Neven 1987) 1.7 21d, Daphnia magna (van Leeuwen et al. 1987) 2 23d, Daphnia magna (Beusen & Neven 1987)
EC50 values to crustaceans, mg/l	42 2d, mbt, Crangonyx pseudogracilis 12.3 4d, mbt, Crangonyx pseudogracilis (Martin & Holdich 1986) 1.5 Daphnia magna (van Leeuwen et al. 1987) 2.9–4.0 2d, mbt Daphnia magna (Beusen & Neven 1987)
LC50 values to fishes, mg/l	8.0–19.4 2d, Branchydanio rerio 2.9–5.3 4d, Branchydanio rerio 2.3 7d, Branchydanio rerio 14.2 2d, Poecilia reticulata 17.1 2d, Poecilia reticulata 10.2 4d, Poecilia reticulata 6.1 4d, Poecilia reticulata 3.3 7d, Poecilia reticulata (Beusen & Neven 1987)

1806 • Solvent Red-24 85-83-6

Sumformula of the chemical	C24H20N4O
EINECS-number	2016358
Melting point, °C	184–185 (MITI 1992)
Bioconcentration factor, fishes	< 0.29–2.9 6w, Cyprinus carpio, conc 0.35 mg/l < 2.9–11 6w, Cyprinus carpio, conc 0.035 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	> 100 48hr, Oryzias latipes (MITI 1992)

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1807 • Sorbitan lauric acid monoester 1338-39-2

Synonyms	Sorbitan monolaurate Sorbitan, monododecanoate
Sumformula of the chemical	C18H3406
EINECS-number	2156633
Total degradation in water	Biodegradation: 56.9% by BOD (on the upward trend) period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

1808 • Sorbitan oleic acid monoester 1338-43-8

Synonyms	Sorbitan, mono-9-octadecenoate, (Z)- Sorbitan monooleate Sorbitan oleate
Sumformula of the chemical	C24H4406
EINECS-number	2156654
Total degradation in water	Biodegradation: 57.9% by BOD (on the upward trend) period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

1809 • Sorbitan palmitic acid monoester 26266-57-9

Sumformula of the chemical	C22H4206
Total degradation in water	Biodegradation: 52.4% by BOD (on the upward trend) period: 21d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

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1810 • Stannous chloride 7772-99-8

LC50 values to crustaceans, mg/l	37 19.5	1d, Daphnia magna 2d, Daphnia magna (Khangarot et al. 1987)
EC50 values to crustaceans, mg/l	71.8 50.1	2d, mbt, Crangonyx pseudogracilis 4d, mbt, Crangonyx pseudogracilis (Martin & Holdich 1986)

1811 • Stearic acid

57-11-4

Sumformula of the chemical	C18H36O2	
Molecular weight	284.47	
Water solubility, mg/l	340	25 °C (Suntio et al. 1988)
Melting point, °C	69–70	(Suntio et al. 1988)
LC50 values to fishes, mg/l	14	act, Poecilia reticulata (Bock 1967)

1812 • Strobane

8001-50-1

LC50 values to fishes, mg/l	0.05	48hr, Lepomis cyanellus (Kemp et al. 1973)

1813 • Strychnine

57-24-9

LC50 values to fishes, mg/l	0.87 0.95	96hr, Lepomis macrochirus 96hr, Menidia audens (Dawson et al. 1977)

1814 • Strychnine sulfate

60-41-3

Other information about mammals	ALD = 8.0 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987).	
LD50 values to birds in oral exposure, mg/kg	6 5 5.62 ≥ 10.0	orl-Agelaius phoeniceus orl-Sturnus vulgaris orl-Carpodacus mexicanus orl-Turdus migratorius (Schafer et al. 1983)

1815 • Styrene

100-42-5

Synonyms	Vinylbenzene Ethenylbenzene Phenethylene Phenylethene Phenylethylene Styrol Styrole Styrolene Vinylbenzol Cinnamene Cinnamol
Sumformula of the chemical	C8H8
Use	Manufacturing of polystyrene, synthetic rubber, ABS plastics; manufacturing of resins, insulators, protective coatings. Monomer for plastic production.
State and appearance	Colourless, viscous liquid.

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Odour	Pungent odour. Threshold odour concentration in water: < 1 mg/l (Fawell & Hunt 1988). Quality: sharp, sweet Hedonic tone: unpleasant Threshold odour concentration absolute: 0.05 ppm 50% recognition: 0.15 ppm 100% recognition: 0.15 ppm Odour index 100% recognition: 44 391 (Hellman & Small 1974).
Molecular weight	104.16
Vapour density (air=1)	3.6
Conversion factor, 1 ppm in air=	4.2 mg/m3
Conversion factor, 1 mg/m³ in air=	0.24 ppm
Vapour pressure, mmHg	5 20 °C 10 30 °C 6.6 25 °C, extrapolated (Boublik et al. 1984)
Water solubility, mg/l	300 20 °C 310 25 °C (Yalkowsky 1987)
Melting point, °C	-30.63
Boiling point, °C	145.2 (MITI 1992)
Log octanol/water coefficient, log Pow	2.95 (Anon. 1988) 2.95 (Hansch & Leo 1985) 3.05 (Sangster 1989)
Henry's law constant, Pa x m³/mol	230 (Anon. 1988) 285 estimated (Hine & Mookerjee 1975) 266.8 calc. (Yaws et al. 1991)
Volatilization	Relative volatility (nBuAc=1) = 0.52 The volatilization half-life of styrene from a model river one m in depth with water current speed of one m/sec and wind velocity of 3 m/sec is calculated to be about 3 hours. (Lyman et al. 1982)
Adsorption/desorption	Relatively strong adsorption observed in a sand aquifer as breakthrough time took about 80 times longer than a nonadsorbing tracer. (Roberts et al. 1980) Estimation of Koc from a water solubility of 160 ppm yields a Koc value of about 270. (Banerjee et al. 1980, Lyman et al. 1982) Estimation of Koc from log Kow 2.95 yields a Koc value of about 550. (Harkov et al. 1985, Lyman et al. 1982) Koc values of 270–550 indicate moderate to low soil mobility. (Swann et al. 1983)
Mobility	Equilibrium distribution: *mass %* air 98.60 water 1.23 solid 0.17 (Anon. 1988).
Other physicochemical properties	Soluble in ethanol, diethylether and acetone; very soluble in benzene and petroleum ether.

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Photochemical degradation in air	Styrene vapour in the atmosphere will react rapidly with hydroxyl radicals and with ozone. The reaction half-lives of styrene with hydroxyl radicals and ozone are calculated to be 3.5 and 9 hours, respectively. (Atkinson & Carter 1984, Bignozzi et al. 1981) Styrene does not absorb solar radiation; therefore, it should not be directly photolyzed in the troposphere or surface water. However, it is a very active generator of photochemical smog due to indirect photochemical reactions. (Darnell 1976)
Chemical oxygen demand, g 02/g	2.8 5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	1.29 5 days (Bridie et al. 1979)
Total degradation in water	Biodegradation: 100% by BOD period: 14d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
Other information about degradation	95% styrene degradation from a landfill soil and 87% degradation from a sandy loam soil in 16 weeks as measured by C02 evolution. (Sielicki et al. 1978) Degradation of 2.3–12% per week has been observed with two su subsurface aquifers. (Wilson et al. 1983) Five-day aqueous theoretical BOD (TBOB) of 80% in acclimated sewage seed and 42% TBOD in an unacclimated seed have been observed. (Bridie et al. 1979) Five-day aqueous TBOD was 65% and 2-day TBOD was 87% with a filtered sewage seed, but TBOD's dropped to 8% (5-day) and 80% (20-day) in salt water. (Price et al. 1974) In 17 days of incubation using a sewage seed, C02 production reached about 20% of theoretical. (Pahren & Bloodgood 1961) Styrene was degraded in mixed propane-utilizing bacteria isolated from soil and lakes, with styrene oxide formed as a product. (Hou et al. 1983)
Metabolism in mammals	The results of controlled laboratory studies on animals and human beings have shown that uptake of styrene is rapid and that it is widely distributed throughout the body. Uptake is mainly via the pulmonary and, to a lesser extent, the dermal and oral routes (WHO 1983). Styrene is distributed through the whole body and stored in lipid depots. Its subsequent slow elimination from the tissue indicates a potential for bioaccumulation following repeated daily exposure (WHO 1983). Styrene is biotransformed largely via the 7,8-epoxide by the mixed function oxidase system. The principal urinary metabolites are α-hydroxybenzeneacetic (mandelic) and phenylglyoxylic acids. Recent evidence suggests that the pattern of urinary metabolite excretion varies with mammalian species. Other minor metabolic pathways may also be important in the toxicological assessment of this compound (WHO 1983). The elimination of styrene and its metabolites appears to involve a two-compartment kinetic model that becomes monophasic in experimental animals at high exposure levels. This suggests the existence of saturable metabolic pathways (WHO 1983). Exposure levels can be assessed by the quantitative analysis of alveolar air or determination of the urinary metabolites, mandelic and phenylglyoxylic acid. At present, urinary mandelic acid appears to be the most reliable biological indicator of exposure in human beings (WHO 1983)
Bioconcentration factor, fishes	13.5 Carassius auratus (Ogata et al. 1984)

LD50 values to mammals in oral exposure, mg/kg	5000 316 1000	orl-rat orl-mus (Lewis & Sweet 1984) orl-rat (Verschueren 1983)
LD50 values to mammals in non-oral exposure, mg/kg	660 1220 90	ipr-mus ipr-rat ivn-mus (Sweet 1987)
LC50 values to mammals in inhalation exposure, mg/m³	21600 24000	ihl-mus ihl-rat, 4hr (Sweet 1987)
LCLo values to mammals in inhalation exposure, mg/kg	12000	ihl-gpg, 14hr (Sweet 1987)
LCLo values to mammals in inhalation exposure, ppm	10000	ihl-hmn, 30 min (Sweet 1987)
TDLo values to mammals in oral exposure, mg/kg	8600 5575 6000	orl-rat, 1–22d preg. effects on newborn orl-rat, multigenerations effects on newborn orl-rat, effects on newborn (Sweet 1987)
TCLo values to mammals in inhalation exposure, mg/kg	1.5 5 1.5	ihl-rat, 24hr, 1–22d preg. effects on embryo or fetus ihl-rat, 24hr, 1–22d preg. effects on newborn ihl-rat, 24hr, 1–7d preg. effects on fertility (Sweet 1987)
TCLo values to mammals in inhalation exposure, ppm	600 1000 500 300 600 0.02	ihl-hmn (Lewis & Sweet 1984) ihl-ham, 6hr, 6–18d preg. effects on fertility ihl-mus, 6hr, 6–16d preg. effects on fertility ihl-rat, 7hr, 6–15d preg. effects on embryo of fetus maternal effects nutritional and gross metabolic ihl-hmn, sense organs and special senses ihl-hmn, sense organs and special senses (Sweet 1987)
Effects on the reproduction of mammals	Results of a few studies on mammals (rats, mice, and Chinese hamsters) suggest that inhaled styrene has embryotoxic effects. Only a limited number of studies on women are available, with inconclusive results (WHO 1983).	
Other information about mammals	Skin and eye irritation data: skin, human, 500 mg nse; skin, rabbit, 500 mg open, mild; skin, rabbit, 100%, moderate; eye, rabbit, 18 mg (Sweet 1987).	

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Health effects	Exposure levels of 420 mg/m³ (100 ppm) and above cause irritation of the mucous membranes of the eyes and the upper respiratory tract in man. Similar effects have been observed in experimental animals. Exposure of human volunteers to levels exceeding 840 mg/m³ (200 ppm) resulted in drowsiness, nausea, and disturbed balance, within a few minutes. Prolonged reaction times have been reported in connection with short-term exposure of human volunteers to 840 mg/m³ (WHO 1983). Epidemiological studies on workers with long-term occupational exposure to styrene have shown an increased prevalence of abnormal EEGs associated with urinary mandelic acid concentration of 700 mg/l or more; at 1600 mg/l, a reduction in psychomotor performance and visuomotor accuracy in psy evidence of adverse effects on the peripheral nervous system is still not available (WHO 1983).
Carcinogenicity	NCI carcinogenesis bioassay completed: results negative: mus, rat (Lewis & Sweet 1984). Several case reports and epidemiological studies have implied an increased risk of cancers of the lymphatic and hematopoietic systems in workers involved in the manufacture of styrene and polystyrene and styrene-butadiene rubber. However, at present there is insufficient evidence to establish a direct cause and effect relationship between styrene exposure and cancer in human beings (WHO 1983). A single experimental study in mice indicated limited evidence for the carcinogenicity of styrene in this species. Orally administered styrene 7,8-oxide, the primary metabolite of styrene, was carcinogenic in rats (WHO 1983).
Mutagenicity	When metabolically activated, styrene may be mutagenic and clastogenic in many experimental systems. Conflicting results obtained in some in vitro mutagenicity assays, were presumably due to differences in metabolic activation and inactivation of styrene. Styrene 7,8-oxide is the main reactive intermediate of styrene biotransformation. It is an alkylating agent that is mutagenic and clastogenic in many in vitro test systems (WHO 1983). Several studies have indicated an increased frequency of structural chromosome aberrations in the peripheral blood lymphosytes of workers exposed to styrene in the reinforced plastics industry. Negative results have been reported in workers employed in the production of styrene monomer and polystyrene, where exposure to styrene is lower (WHO 1983). Because of complexity of the evaluation of the total exposure of workers in the reinforced plastics industry, it has not been possible to show, unequivocally, that styrene is the cause of the observed somatic chromosome aberrations. Even though the biological and health significance of somatic chromosome damage is not understood at present, the increase in such effects is considered to be an indicator of possible adverse health effects (WHO 1983). Mutation data: cytogenetic analysis: ham, lug, 100 mg/l; hmn, lym, 300 ppm, 72hr; rat, ihl, 300 ppm; DNA damage: mus, ipr, 10 mmol/kg; rat, liver, 3 mmol/l; DNA inhibition: hmn, hla, 28 mmol/l; unscheduled DNA synthesis: hmn, lym, 0.1 mmol/l; gene conversion and mitotic recombination: smc, 1 mmol/l; host-mediated assay: mus, smc, 1000 mg/kg; mus, ssp, 1000 mg/kg; gene mutation in mammalian cells: ham, lug, 0.240 mmol/plate; micronucleus test: mus-ipr, 250 mg/kg; microbial mutation without S9: smc, 1 mmol/l; microsomal assay: sat, 1 µmol/plate; oncogenic transformation: rat, emb, 0.145 mg/plate; sister chromatid exchange: hmn, lym, 0.5 mmol/l; mus, ihl, 46.4 mg/kg; mus, ihl, 125 ppm (Sweet 1987).

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Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 72 mg/l (Bringmann & Kühn 1980a)
LOEC values to algae, mg/l	67 rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to crustaceans, mg/l	23 48hr, Daphnia magna (LeBlanc 1980) 68 24hr, Artemia salina (Pickering & Henderson 1966)
LC50 values to fishes, mg/l	9.1 96hr, Cyprinodon variegetus (Heitmuller et al. 1981) 25 96hr, Lepomis macrochirus (Pickering & Henderson 1966) 26 24hr, Carassius auratus (Bridie et al. 1979)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): > 200 mg/l protozoa (Entosiphon sulcatum): > 256 mg/l (Bringmann & Kühn 1980a)

1816 • Styrene oxide 96-09-3

Sumformula of the chemical	C8H8O
EINECS-number	2024767
Melting point, °C	< -10 (MITI 1992)
Boiling point, °C	191–192 (MITI 1992)
Total degradation in water	Biodegradation: 80–82% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

1817 • Sulfite 14265-45-3

LC50 values to fishes, mg/l	5.7 96hr, pugnose minnow (Ward & DeGraeve 1978)

1818 • Sulfolane 126-33-0

Synonyms	Thiocyclopentane-1,1-dioxide Tetramethylenesulfone Sulfoxaline Dihydrobutadienesulfone Tetrahydrothiophene-1,1-dioxide
Melting point, °C	27 (MITI 1992)
Boiling point, °C	285 (MITI 1992)
Chemical oxygen demand, g O2/g	1.75 5 days (Bridie et al. 1979)
Biochemical oxygen demand, g O2/g	0 5 days (Bridie et al. 1979)

ST

Total degradation in water	Biodegradation: 10.1% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 1.3 < 13	6w, Cyprinus carpio, conc 2.5 mg/l 6w, Cyprinus carpio, conc 0.25 mg/l (MITI 1992)
LC50 values to fishes, mg/l	4800 2450	24hr, Carassius auratus (Anon. 1975) 48hr, Oryzias latipes (MITI 1992)

1819 • Sulfotep

3689-24-5

Synonyms	0,0,0',0'-Tetraethyldithiopyrophosphate TEDP	
Use	Active ingredient in insecticides; acaricide.	
Molecular weight	322.34	
Vapour pressure, mmHg	0.00017	20 °C
Water solubility, mg/l	25–66	room temperature
Boiling point, °C	138	
LD50 values to mammals in oral exposure, mg/kg	5 3	orl-rat, orl-dog orl-cat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	20	skn-rbt (Lewis & Sweet 1984)
LC50 values to mammals in inhalation exposure, mg/m³	38	4hr, ihl-rat (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	24 100 < 100 100	orl-ckn orl-bwd (Lewis & Sweet 1984) orl-Agelaius phoeniceus orl-Sturnus vulgaris (Schafer et al. 1983)
LC50 values to crustaceans, mg/l	0.00023	48hr, Daphnia sp. (Meier et al. 1979)
LC50 values to fishes, mg/l	0.018 0.0016 0.18	96hr, Salmo gairdneri 96hr, Lepomis macrochirus 96hr, Pimephales promelas (Meier et al. 1979)

1820 • Sulfur chloride

10025-67-9

Synonyms	Sulfur monochloride Sulfur subchloride Disulfur chloride Chlorosulfane Thiosulfurous dichloride
Sumformula of the chemical	Cl2S2
Use	Chemicals production; fungicides; insecticides; rubber synthesis; dyes.

State and appearance	Light amber to yellowish red, fuming, oily liquid. Will evolve gas; will be present as H2S, sulfur, sulfite, thiosulfuric acid, and HCl.
Odour	Penetrating odour. Recognition odour 0.001 ppm in air (Sax 1986).
Molecular weight	135.03
Specific gravity (water=1)	1.69
Vapour pressure, mmHg	10 at 40 °C
Melting point, °C	-80
Boiling point, °C	135.6
Other information about degradation	Decomposes on contact with water (Sax 1986).
Health effects	Vapours irritate; cause tears in eyes. Affects breathing. Corrosive vapours affect eyes, lungs, and mumem. Vapours decompose in lung moisture to corrosive products (Sax 1986). Acute hazard level: Strong irritant. Highly toxic when ingested or inhaled. A concentration of 150 ppm in air has been fatal to mice in 1 M (Sax 1986). Chronic hazard level: Moderately toxic with ingestion or inhalation (Sax 1986).
Effects on plants	Chronic plant toxicity limit: 350 ppm (Sax 1986).
Other information about water organisms	Regarding freshwater and saltwater toxicity tests see H2S, sodium sulfite and thiosulfite.
Other information	Emits toxic vapours when contacted with acid or water, or when heated to decomposition (Sax 1986).

1821 • Sulfur dioxide 7446-09-5

Synonyms	Bisulfite Sulfurous acid anhydride Sulfurous anhydride Sulfurous oxide Sulfur oxide	
Sumformula of the chemical	02S	
Molecular weight	64.06	
LC50 values to mammals in inhalation exposure, ppm	3000 2520	ihl-mus, 30min ihl-rat, 1hr (Sweet 1987)
LCLo values to mammals in inhalation exposure, ppm	1039 1000 3000 3000	ihl-gpg, 24hr ihl-hmn, 10min ihl-hmn, 5min ihl-mam, 5min ihl-gpg, 24hr ihl-hmn, 10min ihl-hmn, 5min ihl-mam, 5min ihl-gpg, 24hr ihl-hmn, 10min ihl-hmn, 5min ihl-mam, 5min ihl-gpg, 24hr ihl-hmn, 10min ihl-hmn, 5min ihl-mam, 5min (Sweet 1987)

ST

TCLo values to mammals in inhalation exposure, mg/kg	4	ihl-rat, 24hr, 72d preg. maternal eff., eff. on fertility effects on newborn
	4.97	ihl-rat, 12hr, 12w preg., maternal eff. effects on newborn (Sweet 1987)
TCLo values to mammals in inhalation exposure, ppm	25	ihl-mus, 6-15d preg., 7hr
Other information about mammals	Skin and eye irritation data: eye, rabbit, 6 ppm, 4hr, 32 d, mild (Sweet 1987).	
Mutagenicity	Mutation data: cytogenetic analysis: cattle, cell types, 2.5 mmol/l; domestic animal, cell types, 5 mmol/l; DNA damage: hmn, lym, 5700 ppb; DNA inhibition: hmn, lym, 5700 ppb; microbial mutation without S9: microorganisms, 10 mmol/l; smc, 5 µmol/l; sex chromosome loss and nondisjunction: dmg, orl, 0.2 mmol/l (Sweet 1987).	
Effects on amphibia	LCLo, ihl, frog, 15 min, 1 pph (Sweet 1987).	

1822 • Sulfur Green-14

12227-06-4

Water solubility, mg/l	62	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.3–22	6w, Cyprinus carpio, conc 1 mg/l
	< 3.2–9.4	6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 200	48hr, Oryzias latipes (MITI 1992)

1823 • Sulfuric acid

7664-93-9

Synonyms	Vitriol Hydrogen sulfate Vitriolic acid
Sumformula of the chemical	H2SO4
Purity, %	65–100%
Use	Fertilizers; chemicals; inorganic pigments; petroleum refining; etchant; alkylation catalyst; rayon and film; industrial explosives; nonferrous metallurgy; parchment paper.
State and appearance	Colourless liquid. Will sink and dissolve. Spend sulfuric acid is a black oily liquid.

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Odour	Odour threshold; lower 0.6–1.0 mg/m³ (Sax 1986). Sharp penetrating odour.	
Molecular weight	98.08	
Specific gravity (water=1)	1.834	
Vapour pressure, mmHg	1	145.8 °C
Melting point, °C	3	for 98.3%
Boiling point, °C	338	for 98.3%
Other physicochemical information	Potential for accumulation negative. Natural alkalinity will slowly neutralize (Sax 1986).	
LD50 values to mammals in oral exposure, mg/kg	2140	orl-rat (Sax 1986)
LC50 values to mammals in inhalation exposure, mg/m³	18 500 50 320 510	8hr, gpg babies, ihl 8hr, ihl-mus 8hr, ihl-gpg (Sax 1986) 2hr, ihl-mus 2hr, ihl-rat (Sweet 1987)
LCLo values to mammals in inhalation exposure, mg/kg	500 549 165	ihl-rat ihl-mus ihl-mus (Sax 1986)
LCLo values to mammals in inhalation exposure, ppm	178 140 48	7hr, ihl-rat 3.5hr, ihl-rat, ihl-gpg 7hr, ihl-rat 3.5hr, ihl-rati, hl-gpg 7hr, ihl-rat 3.5hr, ihl-rat, ihl-gpg (Sax 1986)
TCLo values to mammals in inhalation exposure, mg/kg	3	24w, ihl-hmn (Sax 1986)
Other information about mammals	Skin and eye irritation data: eye, rabbit, 1.38 mg, severe; eye, rabbit, 100 mg rinse, severe (Sweet 1987).	
Health effects	Extremely irritative, corrosive, and toxic to tissues, no systemic effects following continual ingestion of small amounts. Repeated contact with dilute solutions can cause dermatitis. Repeated or prolonged inhalation can cause inflammation of the upper respiratory tract, leading to chronic bronchitis. 0.125 to 0.50 ppm can be mildly annoying; 1.5 to 2.5 ppm can be definitely unpleasant; and 10 to 20 ppm is unbearable. Sensitivity to mists and vapours varies with the individual. Workers gradually lose their sensitivity to low concentrations (Sax 1986). Eye, nose, and throat irritation; anuria; bronchitis; conjunctivitis; corneal necrosis; dental erosion and discolouration; dermatitis; emphysema; hemoptysis; nausea and vomiting; pneumonitis; pulmonary edema; stoma titis; skin and eye burns (Sax 1986). As little as 1 oz may cause death (Sax 1986). Extremely corrosive. A hazard by all contact routes. A moderate chronic hazard with inhalation or contact. Emits toxic vapours when heated to decomposition (Sax 1986).	
Effects on wastewater treatment	58 ppm caused 50% inhibition of sewage organisms. May drop pH to levels too low for coagulation (Sax 1986).	

LC50 values to crustaceans, mg/l	60–70 90 80–90	48hr, Crangon crangon (Kemp et al. 1973) 48hr, crab 48hr, shrimp (Sax 1986)
LC50 values to fishes, mg/l	100–330	48hr, Platichthys flesus (Kemp et al. 1973)
Other information about water organisms	Lethal: 1000 mg/l, 0.5–75hr, goldfish, hrd; 138 mg/l, 5–6hr, goldfish, sfd; 50 mg/l, 1–3hr, Daphnia magna, sfd; 1.2 mg/l, sunfish; 24.5 mg/l, 24hr, bluegills; 80.1 mg/l, whitefish; 38 mg/l, 24hr, Daphnia magna, sfd; 10 mg/l, 168hr, Daphnia magna, sfd; 0.1 mg/l, 168hr, Daphnia magna, sfd; 30 mg/l, 24hr, Daphnia magna, sfd (Sax 1986). Harmful: 29 mg/l, 24–72hr, Daphnia magna, sfd, pH 5; 33.11 mg/l, bivalve larvae, sfd, pH 5; 50 mg/l, all aquatic life; 88 mg/l, 64hr, Daphnia magna; 138 mg/l, Daphnia magna (Sax 1986). Toxic threshold: 0.63 mg/l, Polycelis nigra. pH 3.2 (Sax 1986).	
Other information	The toxicity of sulfuric acid is based on the acidity and thus is dependent on the buffer capacity of dilution water. Hydrolysis product of chlorosulfuric acid (Sax 1986). Reacts with many metals giving off hydrogen gas (Sax 1986). Miscible with HOH (Sax 1986).	

1824 • Sumicidin * 51630-58-1 (Fenvalerate)

Active ingredients	Fenvalerate * 200 g/l	
LC50 values to crustaceans, mg/l	0.0019	96hr, 21 °C, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	0.002–0.003	96hr, 10 °C, Alburnus alburnus (Linden et al. 1979)

1825 • 2,4,5-T 93-76-5

Synonyms	2,4,5-Trichlorophenoxyacetic acid	
Use	Herbicide, to control woody plants.	
Molecular weight	255.48	
Water solubility, mg/l	278	25 °C
Melting point, °C	158	
Half-life in soil, days	33	(Li et al. 1990)
Total degradation in soil	Biodegradation: > 205 days for ring cleavage in soil suspension. 75–100% disappearance from soils: 5 months (Verschueren 1983).	

ST

Bioconcentration factor, fishes	26	32 d, Bambusia affinis (Verschueren 1983)
LD50 values to mammals in oral exposure, mg/kg	300 100	orl-rat orl-dog (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	310	orl-ckn (Lewis & Sweet 1984)
Effects on plants	Aspen plants (Populus tremula) were grown in 0.000001 M 2,4,5-T solution → necrosis on the leaves, time of survival 24 days (Eliasson 1963).	
EC50 values to algae, mg/l	50 50	10d, rpd, schr, Isochyris galbana 10 d, rpd, Phaedactylum tricornutum (Walsh 1972)
LC50 values to crustaceans, mg/l	0.73 5 55	act, Daphnia pulex (Nishiuchi & Hashimoto 1967) 96hr, Daphnia magna (Knapek & Lekola 1974) 96hr, Daphnia magna (Kenaga 1979)
LC50 values to fishes, mg/l	0.15 16.4 28.1 8.7 0.15 5.3 0.87 12	96hr, Salmo gairdneri (Yockim et al. 1978) 96hr, Perca fluviatilis 96hr, Poecilia reticulata (Rehwoldt et al. 1977) acetone liquid, 96hr, Salmo gairdneri emulsion, 96hr, Salmo gairdneri (Yokote et al. 1977) 96hr, Cyprinus carpio (Knapek & Lekola 1974) 48hr, Cyprinus carpio (Nishiuchi & Hashimoto 1967) act, Salmo gairdneri (Kenaga 1979)

1826 • TCDD 1746-01-6

Synonyms	2,3,7,8-Tetrachlorodibenzo-1,4-dioxine 2,3,7,8-Tetrachlorodibenzo-p-dioxine	
Sumformula of the chemical	$C_{12}H_4Cl_4O_2$	
Molecular weight	321.97	
Density, kg/m³	1830	20 °C
Water solubility, mg/l	0.0002	22 °C
Melting point, °C	322 305–307	
Boiling point, °C	900	approx.
Degradation point, °C	> 750	
Log octanol/water coefficient, log Pow	7.1 6.8	
Henry's law constant, Pa x m³/mol	7.26	25 °C
Photochemical degradation in water	Water solubility in sun light: half-life 6.3–8 days (Corbet et al. 1988).	
Half-life in soil, days	730–1095d = 2–3y, Seveso (Heckel 1984)	
Half-life in water, days	600	aquatic model ecosystem (Verschueren 1983)
Total degradation in water	Half-life in aquatic model ecosystem: approx. 600 days (Verschueren 1983).	

Total degradation in sediment	In lake sediment no remarkable degradation (Czuczwa & Hites 1984).
Other information about degradation	Quick photochemical degradation in laboratory experiment (Rappe 1980). Degradation only with high microbial activity if TCDD is in bioavailable form (Corbet et al. 1988).
Metabolism in mammals	Uptake in alimentary canal very effective (≥ 80%) (Jones & Bennett 1989). Man, estimated half-life approximately 5 years (Jones & Bennett 1989).
Metabolism in fishes	Half-life, Salmo gairdneri, 15–48 days (Mehrle et al. 1988). Half-life, carp, > 300 days (Kuehl et al. 1986).
Bioconcentration factor, fishes	26700 28d, Salmo gairdneri 39000 static, Salmo gairdneri (Mehrle et al. 1988)
Bioconcentration factor, mollusca	1400–47000 mussel (Vershueren 1983)
Bioconcentration factor, algae	200–18600 algae (Verschueren 1986)
LD50 values to mammals in oral exposure, mg/kg	0.02 orl-rat (Rippen 1988) 0.0006 orl-gpg (NIOSH 1979) 0.0042 orl-mink (Hochstein et al. 1988)
LD50 values to mammals in non-oral exposure, mg/kg	0.0006–0.002 ukn-gpg 1–5 ukn-ham (Virtanen & Nuuja 1987)
Other information about mammals	Rat, NOAEL, 0.000001 mg/kg/day (Rippen 1988). Rhesus ape, oral, 20 months, toxic effects e.g. teratogenic and embryotoxic effects, 0.0000016 mg/kg/day (Rippen 1988).
Health effects	Man, tolerable daily intake, 1–5 pg/kg (Tarkowski & Yrjänheikki 1986).
Carcinogenicity	Very effective tumor promoter (Rippen 1988). Possibly carcinogenic (Holder & Menzel 1988).
Mutagenicity	Not proved to be mutagenic (Rippen 1988).
LD50 values to birds in oral exposure, mg/kg	0.025–0.05 orl-chicken (Rippen 1988)
LOEC values to fishes, mg/l	0.000001 srv, grw, schr, Salmo gairdneri (Helder 1981) 0.000001 srv, grw, chr, Esox lucius (Helder 1980)
NOEC values to fishes, mg/l	0.0000001 srv, grw, schr, Salmo gairdneri (Helder 1981) 0.0000001 srv, grw, chr, Esox lucius (Helder 1980)
Other information about water organisms	Salmo gairdneri, juvenile, survival, growth, behaviour, 28 + 28 days, < 0.000000038 mg/l (Mehrle et al. 1988). Oncorhynchus kisutch, 96hr, 30 d, 55% mortality, 0.0000056 mg/l (Miller et al. 1979).

1827 • 2,4,5-TCPPA

93-72-1

Synonyms	2,4,5-Trichlorophenoxypropionic acid
EC50 values to algae, mg/l	25 10d, rpd, Chlorococcum sp. Dunaliella terticulata 5 10d, rpd, Isochyris galbana (Walsh 1972)

ST

LC50 values to crustaceans, mg/l	2,4,5-TCPPA butoxyethyl ether:	
	0.25	96hr, Gammarus fasciatus
	2.1	48hr, Daphnia magna
	4.9	48hr, Cypridopsis vidua (Sanders 1970)
	2,4,5-TCPPA propyleneglycolbutylester:	
	0.18	48hr, Daphnia magna
	0.2	48hr, Cypridopsis vidua (Hughes & Davis 1963)
LC50 values to fishes, mg/l	83	48hr, Lepomis macrochirus (Hughes & Davis 1963)
	0.35	96hr, Gambusia affinis (Gupta et al. 1979)
	2,4,5-TCPPA butoxyethyl ether:	
	1.1	48hr, Lepomis macrochirus (Sanders 1970)
	2,4,5-TCPPA isooctyl ester:	
	16	48hr, Lepomis macrochirus (Hughes & Davis 1963)
	2,4,5-TCPPA propyleneglycolbutylester:	
	16.6	48hr, Lepomis macrochirus (Hughes & Davis 1963)

1828 • Tellurium and tellurium compounds 13494-80-9

Sumformula of the chemical	Te	
Molecular weight	127.6	
LDLo values to mammals in non-oral exposure, mg/kg	290	scu-dog (Lewis & Sweet 1984)
	200	itr-rat (Lewis & Sweet 1984)
TDLo values to mammals in oral exposure, mg/kg	3465	orl-rat, 1–21 days preg. (Lewis & Sweet 1984)
TDLo values to mammals in non-oral exposure, mg/kg	13	ims-rat,9 days preg. (Lewis & Sweet 1984)
LC50 values to fishes, mg/l	21.6	28d, Salmo gairdneri (Birge et al. 1980)

1829 • Terbutryne 886-50-0

Synonyms	2-(tert-Butylamino)-4-(ethylamino)-6-(methylthio)-s-triazine N-tert-Butyl-N-ethyl-6-methylthio-1,3,5-triazine-2,4-diyldiamine	
Use	Active ingredient in herbicides.	
Molecular weight	241.6	
LD50 values to mammals in oral exposure, mg/kg	2500	orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	2900	unk-mam (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	4000	orl-ckn (Lewis & Sweet 1984)
Effects on plants	3.0 kg terbutryn/ha was applied with a sprayer following seeding (preemergence) to lamb's-quarters (Chenopodium album) → atrazine-susceptible plants (seeds) were killed and there was a decrease in shoot growth and plant number of atrazine- resistant plants (Jensen et al. 1977).	
LC50 values to crustaceans, mg/l	1.4	48hr, Daphnia magna (Tyson 1974)

ST

LC50 values to fishes, mg/l	4	96hr, Lepomis macrochirus
	1.4–4.0	96hr, Cyprinus carpio
	1.8–3.0	96hr, Salmo gairdneri
		(Pesticide Manual 1983)

1830 • Terbutylazine

5915-41-3

Synonyms	Terbutylazin N-tert-Butyl-6-chloro-N'-ethyl-1,3,5-triazine-2,4-diamine Faneron Combi 500 FW * Gardoprim-liquid * 4-tert-Butylamino-2-chloro-6-ethylamino-s-triazine 2-tert-Butylamino-4-chloro-6-ethylamino-s-triazine
Sumformula of the chemical	$C_9H_{16}ClN_5$
Products containing the chemical	Faneron Combi 500 FW * Bromophenoxim 330 g/l Terbutylazine 170 g/l (PESREG) Gardoprim-liquid * Terbutylazine 500 g/l (PESREG)
Use	Active ingredient in herbicides.
State and appearance	White powder. Flowable water based suspension. (Gardoprim-liquid *) (PESREG)
Molecular weight	229.75
Density, kg/m³	1188 (Esser et al. 1975) 1.09–1.13 g/cm³, at 20 °C, Cardoprim-liquid (PESREG)
Vapour pressure, mmHg	0.0000011 at 20 °C (Esser et al. 1975)
Water solubility, mg/l	5 at 20 °C (PESREG) 8.5 at 20–25 °C (Esser et al. 1975)
Melting point, °C	177–179 (Esser et al. 1975)
pH	7–9 Gardoprim-liquid (PESREG)
pKa	2 at 21 °C (Esser et al. 1975)
Log octanol/water coefficient, log Pow	3.04 at 20 °C, pH 7 (PESREG)
Adsorption/desorption	Adsorption and desorption of terbutylazine was determined in five different soils. The adsorption and desorption coefficients and the adsorption constants were determined.

soil type	*% organic carbon*	*adsorption Ka*	*Koc*	*desorption Kd*
sand	1.4	2.270	162.143	6.966
sand	0.4	1.112	278.000	8.610
sandy loam	1.2	2.355	196.250	9.840
silty loam	3.4	5.943	174.794	17.378
sandy loam	11.2	25.177	224.795	164.816

GLP, EPA (PESREG)

Adsorption cofficient	2.27	sand
	1.112	sand
	2.355	sandy loam
	5.943	silty loam
	25.177	sandy loam
		GLP, EPA (PESREG)

ST

Desorption cofficient	6.966 sand 8.61 sand 9.84 sandy loam 17.378 silty loam 164.816 sandy loam GLP, EPA (PESREG)
Mobility	In the soil columns studies (sandy soil and silty loam, incubated 139 days, and then rainfall 16 days, 12.5 mm daily) of terbutylazine (27.3 ppm) 8.40 and 6.19% of the applied radioactivity were eluted from the soil columns. Most of the aged residues applied to the soil columns were retained in the top 10 cm layers. The main metabolite was 2-chloro-4-amino-6-tert-butylamino-s-triazine. (PESREG) The leaching behaviour of terbutylazine was studied in soil columns (loamy sand, sand, silty loam and sandy loam). The penetration depth of terbutylazine into the soil profile ranged between 6 and 12 cm. GLP, EPA (PESREG) Slightly soluble in organic solvents: dimethylformamide 10% chlorobenzene 1% ethylacetate 4% isopranol 1% methylglycolmonoethylether 4% n-octanol 1.4% xylene 1% (PESREG)
Photochemical degradation in soil	Photolysis of terbutylazine on soils (dry soil and moist soil) was studied under artificial sunlight conditions (24hr). 13 and 15% of used herbicide was degraded in dry and moist soil samples. The main extractable degradation product was 2-hydroxy-4-ethylamino-6-tert-butylamino-s-triazine. (PESREG)
Hydrolysis in water	The half-life of terbutylazine (10 ppm) was > 200 days (pH 7, 50 °C) and 183 days (pH 7, 70 °C). (PESREG) Hydrolysis, pH 5, 25 °C, half-life 63 d; pH 7–9, 25 °C, half-life > 200 d. (Burkhard & Guth 1981) The half-lives of terbutylazine (5 ppm, at 20 °C) have been calculated to be 8 days (pH 1), 12 days (pH 5), > 200 days (pH 7 and 9) and 5 days (pH 13). Under acidic and basic conditions a direct degradation of terbutylazine to 2-hydroxy-4-ethylamino-6-tert-butylamino-s-triazine occurred. (PESREG)
Hydrolysis in acid	The half-life of terbutylazine (10 ppm) was 41 days (pH 5, 30 °C), 12 days (pH 5, 50 °C) and 82 hours (pH 5, 70 °C). (PESREG)
Hydrolysis in base	The half-life of terbutylazine (10 ppm) was > 200 days (pH 9, 50 °C) and 75 days (pH 9, 70 °C). (PESREG)
Half-life in soil, days	84 pH 4.8, 22 °C (Burkhard & Guth 1981) 170 pH 6.5, 22 °C (Burkhard & Guth 1981)
Aerobic degradation in soil	The degradation of terbutylazine (10 ppm) was studied in a silty loam under aerobic conditions. Terbutylazine disappeared with a half-life of about 88 days. The main metabolites were 2-chloro-4-amino-6-tert-butylamino-s-triazine and 2-hydroxy-4-ethylamino-6-tert-butylamino-s-triazine. The formation of 14CO2 was very slow: 1.69% of used herbicide after 225 days (PESREG)
Aerobic degradation in water	The degradation of terbutylazine (1 ppm) was studied in two aquatic (river and pond, both contained 1% of sediment) systems. 80.1% (river) and 79.8% (pond) of used terbutylazine were found after 17.4 weeks of incubation. Half-lives (at 25 °C) were calculated to be 579 days (river) and 463 (pond). The volatile degradation product 14CO2 was found 0.9% (river) and 0.4% (pond) at the end of the experiments. (PESREG)
Total degradation in soil	The degradation of terbutylazine in soil (silty clay soil) was followed under laboratory conditions. N-dealkylation and hydrolysis of the C-2 substituent were the mechanisms for the degradation of terbutylazine. (PESREG)

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Degradation and transformation products	2-chloro-4-amino-6-tert-butylamino-s-triazine 2-hydroxy-4-ethylamino-6-tert-butylamino-s-triazine (PESREG)
Bioconcentration factor, fishes	14.8 28d, 0.402 mg/l, 20-22 °C, edibles 48.6 28d, 0.402 mg/l, 20-22 °C, non-edibles 33.7 28d, 0.402 mg/l, 20-22 °C, whole fish Lepomis macrochirus (GLP, EPA, PESREG)
Other information about bioaccumulation	The bioaccumulation (28d, 20-22 °C) and elimination (in flowing, untreated water 14d) of terbutylazine (0.402 mg/l) by Lepomis macrochirus was investigated in a dynamic flow-through system. *BCF* *half-life (hr)* edibles 14.8 16.3 non-edibles 48.6 22.3 whole fish 33.7 19.2 (GLP, EPA, PESREG)
LD50 values to mammals in oral exposure, mg/kg	1845 orl-rat (Lewis & Sweet 1984) 2000 orl-rat (PESREG) 2160 orl-rat (PESREG) 7700 orl-mus (PESREG) 1346 orl-rat, Gardoprim-liquid (PESREG)
LD50 values to mammals in non-oral exposure, mg/kg	> 3000 idr-rbt (PESREG) 272 ipr-rat (PESREG)
LC50 values to mammals in inhalation exposure, mg/m³	> 3.51 mg/l 4h, ihl-rat (PESREG)
LD50 values to birds in oral exposure, mg/kg	> 1000 orl-bdw, Anas platyrhyncos > 1000 orl-bdw, Coturnix virginianus (PESREG) > 2510 orl-bdw, Anas platyrhynchos (PESREG)
Subacute LC50 values to birds in feeding exposure, mg/kg	> 5620 ppm, 8d, Anas platyrhyncos > 5620 ppm, 8d, Coturnix virginianus (PESREG)
Effects on invertebrates	LC50, 210 mg/kg, 14d, calc., techn., Eisenia foetida LC50, 230 mg/kg, 14d, graph., techn., Eisenia foetida GLP, OECD No 207 (PESREG)
Effects on bees	LD50, 0.020 mg/bee, 20hr, feeding test. LD50, 0.020 mg/bee, 20hr, contact test (PESREG)
EC50 values to algae, mg/l	0.019 5d, grw, Scenedesmus subspicatus 0.02 calc. 5d, grw, Scenedesmus subspicatus (PESREG)
LC50 values to crustaceans, mg/l	21.2 48hr, Daphnia magna (PESREG) 0.092 96hr, techn., Mysidopsis bahia GLP (PESREG)
EC50 values to crustaceans, mg/l	> 3.6 mg/l, 48hr, imb, Daphnia magna 1.8 14d, imb, Daphnia magna 1.1 21d, imb, Daphnia magna 0.9–3.6 mg/l, 14d, 21d, rpd, Daphnia magna GLP, OECD No 202 (PESREG)

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LOEC values to crustaceans, mg/l	3.6 0.9	14d, imb, Daphnia magna 21d, imb, Daphnia magna GLP, OECD No 202 (PESREG)
NOEC values to crustaceans, mg/l	0.9 0.21 0.9	14d, imb, Daphnia magna 21d, imb, Daphnia magna 14d, 21d, rpd, Daphnia magna GLP, OECD (PESREG)
LC50 values to fishes, mg/l	66 52 4.6	96hr, Cyprinus carpio 96hr, Lepomis macrochirus 96hr, Salmo gairdneri (Pesticide Manual 1983)
	4.6 66 7 52 1.6	96hr, Salmo gairdneri 96hr, Carassius carassius 96hr, Ictalurus ameiurus 96hr, Lepomis macrochirus 96hr, Lebistes reticulatus (PESREG)
	3.8 3.6	96hr, techn., calc., Salmo gairdneri 96hr, techn., graph., Salmo gairdneri (OECD No 203, PESREG)
	7 7.2	96hr, techn., calc., Cyprinus carpio 96hr, techn., graph., Cyprinus carpio (OECD No 203, PESREG)

1831 • Terephthalic acid 100-21-0

Synonyms	1,4-Benzenedicarboxylic acid p-Phthalic acid
Sumformula of the chemical	C8H6O4
EINECS-number	2028300
Total degradation in water	Biodegradation: 75% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

1832 • Terephthalic acid, dimethyl ester 120-61-6

Synonyms	1,4-Benzenedicarboxylic acid, dimethyl ester Dimethyl terephthalate
Sumformula of the chemical	C10H10O4
EINECS-number	2044118
Water solubility, mg/l	< 100 (MITI 1992)
Melting point, °C	141–142 (MITI 1992)
Boiling point, °C	288 (MITI 1992)

ST

Total degradation in water	Biodegradation: 84% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

1833 • Terphenyl

26140-60-3

Sumformula of the chemical	C18H14
EINECS-number	2474773
Water solubility, mg/l	> 0.1 (MITI 1992)
Melting point, °C	80–165 (MITI 1992)
Boiling point, °C	350–400 (MITI 1992)
Total degradation in water	Biodegradation: 0.5% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	107–1010 8w, Cyprinus carpio, conc 0.25 mg/l 2–8 8w, Cyprinus carpio, conc 0.25 mg/l 3–15 8w, Cyprinus carpio, conc 0.25 mg/l 502–5480 8w, Cyprinus carpio, conc 0.025 mg/l 9–175 8w, Cyprinus carpio, conc 0.025 mg/l 9–109 8w, Cyprinus carpio, conc 0.025 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	> 50 48hr, Oryzias latipes (MITI 1992)

1834 • α-Terpineol

98-55-5

Melting point, °C	38–40 (MITI 1992)
Boiling point, °C	219–221 (MITI 1992)
Total degradation in water	Biodegradation: 84.6% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
LD50 values to mammals in non-oral exposure, mg/kg	2000 ims-mus (Lewis & Sweet 1984)
LC50 values to fishes, mg/l	10–100 96hr, Salmo gairdneri (Leach et al. 1975)

ST

1835 • Tetrabutoxy titanate 54830-30-7

Sumformula of the chemical	C16H36O4Ti
Melting point, °C	< -40 (MITI 1992)
Boiling point, °C	206 10 mmHg
Total degradation in water	Biodegradation: 84–87% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

1836 • Tetrabutylstannane 1461-25-2

Synonyms	Tetrabutyl tin	
Sumformula of the chemical	C16H36Sn	
Molecular weight	247.21	
Water solubility, mg/l	< 10	(MITI 1992)
Melting point, °C	< -10	(MITI 1992)
Boiling point, °C	289.6–292.5, 760 mmHg (MITI 1992)	
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100mg/l sludge: 30mg/l (MITI 1992).	
Bioconcentration factor, fishes	38–97 127–310	12w, Cyprinus carpio, conc 0.005 mg/l 12w, Cyprinus carpio, conc 0.0005 mg/l (MITI 1992)
LD50 values to mammals in non-oral exposure, mg/kg	56	ivn-mus (Lewis & Sweet 1984)
LDLo values to mammals in non-oral exposure, mg/kg	2000	skn-rbt (Lewis & Sweet 1984)
EC50 values to algae, mg/l	0.017	72hr, grw, Skeletonema costatum (Walsh et al. 1985)
LC50 values to fishes, mg/l	0.723	48hr, Oryzias latipes (MITI 1992)

ST

1837 • 1,1,2,2-Tetrachloro-1,2-difluoroethane 76-12-0

Sumformula of the chemical	C2Cl4F2	
EINECS-number	2009356	
Water solubility, mg/l	190	(MITI 1992)
Melting point, °C	25–27	(MITI 1992)
Boiling point, °C	92.8	(MITI 1992)
Log octanol/water coefficient, log Pow	2.56	(MITI 1992)

Total degradation in water	Biodegradation: 0–37% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992)
Bioconcentration factor, fishes	36–106 6w, Cyprinus carpio, conc 0.05 mg/l 29–90 6w, Cyprinus carpio, conc 0.005 mg/l (MITI 1992)
LC50 values to fishes, mg/l	8.17 48hr (MITI 1992)

1838 • 2,2',3,3'-Tetrachloro-4,4'-diaminodiphenylmethane 42240-73-3

Sumformula of the chemical	C13H10Cl4N
Melting point, °C	165 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Bioconcentration factor, fishes	690–1920 8w, Cyprinus carpio, conc 0.05 mg/l 490–4920 8w, Cyprinus carpio, conc 0.005 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be accumulated on a medium level (Anon. 1987).
LC50 values to fishes, mg/l	1.95 48hr, Oryzias latipes (MITI 1992)

1839 • Tetrachloro-p-benzoquinone 118-75-2

Synonyms	Tetrachloroquinone
Use	Agricultural fungicide; dye intermediate; electrodes for pH measurements; vulcanizing agent.
State and appearance	Yellow leaflets.
Molecular weight	245.9
Specific gravity (water=1)	1.97
Melting point, °C	290
LD50 values to mammals in oral exposure, mg/kg	4000 orl-rat (Nimmo et al. 1979)
Other information about mammals	No ill effects were suffered by rats fed diet containing 0.5% (Verschueren 1983).

1840 • 1,2,3,4-Tetrachlorobenzene 634-66-2

Sumformula of the chemical	C6H2Cl4
Known impurities	1,2,3,5-isomer * technical grade contains 30% 1,2,4,5-isomer

ST

Use	Component of dielectric fluids, synthesis. Byproduct.
State and appearance	Needles.
Odour	Lower odour threshold: 0.006 mg/l in water; lower taste threshold: 0.0064 mg/l (Sax 1986).
Molecular weight	215.88
Water solubility, mg/l	3.5 22 °C 4.31 25 °C (Yalkowsky et al. 1979) 5.92 25 °C (Banerjee 1984) 0.71 (MITI 1992)
Melting point, °C	47.5 45–46 (MITI 1992)
Boiling point, °C	254 (MITI 1992)
Log octanol/water coefficient, log Pow	4.55 (Anon. 1988) 4.72 (Schwarzenbach & Westall 1981) 5.05 (Yalkowsky et al. 1979) 4.46 (Konemann et al. 1979) 4.94 (Konemann et al. 1979) 4.37 (Wateral et al. 1982) 4.55 (Miller et al. 1984) 4.6 (Chiou 1985) 5.02 (MITI 1992)
Log soil sorption coefficient, log Kom	3.83 observed (Sabljic 1987) 3 calculated (Sabljic 1987)
Henry's law constant, Pa x m³/mol	94 (Anon. 1988) 1100 (Suntio et al. 1988)
Mobility	Equilibrium distribution: *mass %* air 83.16 water 2.61 solid 14.22 (Anon. 1988).
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992)
Other information about degradation	Degradation by Pseudomonas (200 mg/l), 30 °C): parent: 33% ring disruption in 120hr mutant: 74% ring disruption in 120hr (Verschueren 1983).
Metabolism in mammals	Six days after rabbits were fed 0.5 g/kg, 5% of the dose was discharged unchanged in the feces; 9.6% was found unchanged in various organs, particularly fat; 5.9% exhaled unchanged; and 42% excreted as metabolites (glucuronide, ethereal sulfate, mercapturic acid, tetrachlorophenol (Sax 1986).
Bioconcentration factor, fishes	2567 32d, Pimephales promelas (USEPA 1984) 524–1540 8w, Cyprinus carpio, conc 0.01 mg/l 489–1710 8w, Cyprinus carpio, conc 0.001 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be accumulated on a medium level (Anon. 1987).

ST

LD50 values to mammals in oral exposure, mg/kg	1167	orl-rat (Lewis & Sweet 1984)
EC50 values to microorganism, mg/l	1.9	15 min Microtox (Hermens et al. 1985)
LC50 values to crustaceans, mg/l	0.32	16d, Daphnia magna (Hermens et al. 1984)
EC50 values to crustaceans, mg/l	0.043	rpd,16d, Daphnia magna (Hermens et al.1984)
NOEC values to crustaceans, mg/l	0.01 0.1	rpd, 16d, Daphnia magna 16d, srv, Daphnia magna (Hermens et al. 1984)
LC50 values to fishes, mg/l	1.1	96hr, Pimephales promelas (Veith et al.1983)
	0.8	14d, Poecilia reticulata (Könemann 1979)
	1.1	4d, Pimephales promelas (Carlson & Kosian 1987)
	1.07	Pimephales promelas (Sax 1986)
	0.365	4d, Poecilia reticulata (Van Hoogen & Opperhuizen 1988)
	1.07	96hr, flow-through, Pimephales promelas (USEPA 1984)
	56	48hr, Oryzias latipes (MITI 1992)
NOEC values to fishes, mg/l	0.245–0.412	32d, Pimephales promelas (USEPA 1984)
Other information about water organisms	0.318 mg/l, chronic value, early life stage test, Pimephales promelas (Sax 1986). LC50, 4 d, 0.00169 mM/l, Poecilia reticulata (Van Hoogen & Opperhuizen 1988).	

1841 • 1,2,3,5-Tetrachlorobenzene 634-90-2

Sumformula of the chemical	C6H2Cl4	
Use	Byproduct.	
Molecular weight	215.88	
Water solubility, mg/l	3.5 5.1 4.02	25 °C (Yalkowsky et al. 1979) 25 °C (Banerjee 1984) 25 °C (Banerjee et al. 1980)
Melting point, °C	50–52 54.5	 (Suntio et al. 1988)
Boiling point, °C	246	
Log octanol/water coefficient, log Pow	4.46–4.94 4.65 5.05 4.52 4.94 4.56 4.51 4.59 4.48	(Sabljic 1987) (Anon. 1988) (Yalkowsky et al. 1979) (Konemann et al. 1979) (Konemann et al. 1979) (Wateral et al. 1982) (Miller et al. 1984) (Chiou 1985) (Hawker & Connell 1985)
Henry's law constant, Pa x m³/mol	400 590 159	(Anon. 1988) calc. (Suntio et al. 1988) exptl. (Suntio et al. 1988)

ST

Mobility	Equilibrium distribution:	
		mass %
	air	94.62
	water	0.69
	solid	4.70
		(Anon. 1988).
Bioconcentration factor, fishes	72000	Poecilia reticulata (Verschueren 1983)
Bioconcentration factor, other organisms	3000	approx. 3000 (Verschueren 1983)
LD50 values to mammals in oral exposure, mg/kg	1727	orl-rat (Lewis & Sweet 1984)
LC50 values to crustaceans, mg/l	9.7	48hr, Daphnia magna (LeBlanc 1980)
LC50 values to fishes, mg/l	3.7	96hr, Cyprinodon variagetus (Heitmuller et al. 1981)
	0.8	14 d, Poecilia reticulata (Könemann 1979)
	6.4	96hr, Lepomis macrochirus (Buccafusco et al. 1981)

1842 • 1,2,4,5-Tetrachlorobenzene 95-94-3

Synonyms	Benzene tetrachloride s-Tetrachlorobenzene	
Sumformula of the chemical	C6H2Cl4	
Use	Manufacture of 2,4,5-trichlorophenol and 2,4,5-trichlorophenoxyacetic acid. Insecticide; impregnant for moisture resistance; electrical insulation; temporary protection in packing; intermediate.	
State and appearance	Needles.	
Molecular weight	215.88	
Specific gravity (water=1)	1.858	
Vapour pressure, mmHg	0.1	
Water solubility, mg/l	0.3	22 °C
	0.595	25 °C (Yalkowsky et al. 1979)
	0.465	25 °C (Banerjee 1984)
	< 1	(MITI 1992)
Melting point, °C	140	(Suntio et al. 1988)
	140	(MITI 1992)
Boiling point, °C	240	(MITI 1992)
Flashing point, °C	155	closed cup
Log octanol/water coefficient, log Pow	4.51	(Anon. 1988)
	4.72	(Schwarzenbach & Westall 1981)
	5.05	(Yalkowsky et al. 1979)
	4.52	(Konemann et al. 1979)
	4.94	(Konemann et al. 1979)
	4.46	(Wateral et al. 1982)
	4.51	(Miller et al. 1984)
	4.7	(Chiou 1985)
	4.98	(MITI 1992)
Log soil sorption coefficient, log Kom	3.86	observed (Sabljic 1987)
	2.99	calculated (Sabljic 1987)

Henry's law constant, Pa x m³/mol	65 (Anon. 1988) 122 calc. (Suntio et al. 1988)
Mobility	Equilibrium distribution: *mass %* air 79.32 water 3.47 solid 17.21 (Anon. 1988).
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992)
Metabolism in mammals	Six days after rabbits were fed 0.5 g/kg, 16% of the dose was discharged unchanged in feces; 48% found unchanged in various organs, primarily fat; 1,6% expired unchanged; and 6.3% excreted as metabolites (glucuronide, ethereal sulfates, tetrachlorophenol) (Sax 1986).
Bioconcentration factor, fishes	2720-4830 8w, Cyprinus carpio, conc 0.01 mg/l 1650-3930 8w, Cyprinus carpio, conc 0.001 mg/l (MITI 1992)
LD50 values to mam-mals in oral exposure, mg/kg	1500 orl-rat 1035 orl-mus (Lewis & Sweet 1984)
EC50 values to algae, mg/l	7.32 96hr, Skeletonema costatum decreased cell number 7.1 96hr, Skeletonema costatum chlorophyll A inhibition 46.8 96hr, Selenastrum capricornutum decreased cell number 52.9 96hr, Selenastrum capricornutum chlorophyll A inhibition (Sax 1986)
LC50 values to crustaceans, mg/l	> 530 48hr, Daphnia magna 1.48 96hr, mysid shrimp (Sax 1986)
LC50 values to fishes, mg/l	0.8 96hr, Cyprinodon variagetus (Heitmuller et al. 1981) 0.3 14 d, Poecilia reticulata (Könemann 1979) 1.6 96hr, Lepomis macrochirus (Buccafusco et al. 1981) 1.55 96hr, Lepomis macrochirus 0.33 96hr, Cyprinodon variegatus (Sax 1986) 26.4 48hr, Oryzias latipes (MITI 1992)
LOEC values to fishes, mg/l	0.18 srv, Cyprinodon variagetus (Ward & Parrish 1980)
Other information about water organisms	0.129 mg/l, chronic value, early life stage test, Cyprinodon variegatus; 0.09 to 0.18 mg/l, > 28 days, estimated maximum acceptable toxicant concentration (Sax 1986).

1843 • Tetrachlorocatechol 1198-55-6

Sumformula of the chemical	C6H2O2Cl4
Molecular weight	247.88

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pKa	3.78	
Log octanol/water coefficient, log Pow	3.7 4.23	 (Xie 1984)
Mobility	0.11% (air), 99.55% (water), 0.34% (sediment)	
LD50 values to mammals in oral exposure, mg/kg	612	orl-mus (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	136	ipr-mus (Lewis & Sweet 1984)
LC50 values to algae, mg/l	0.08	96hr, Selenastrum capricornutum (Kuivasniemi et al. 1985)
EC50 values to algae, mg/l	0.00032	grw, 96hr, Selenastrum capricornutum (Kuivasniemi et al. 1985)
LC50 values to crustaceans, mg/l	3.3	Nitocra spinipes (Renberg et al. 1980)
LC50 values to fishes, mg/l	1.5	96hr, Salmo gairdneri (McKague 1981)
	0.3 0.3	96hr, Salmo salar 96hr, Oncorhynchus gorbusha (Servizi et al. 1966)
	0.8–0.9	Oncorhynchus nerka (Durkin 1978)
	1.1	Salmo trutta (Hattula et al. 1981)
	0.8–0.9	96hr, Salmo salar (Voss et al. 1980)
	0.4	Salmo gairdneri, yearling (Miettinen et al. 1982)
EC50 values to fishes, mg/l	0.01	grw, 96hr, Poecilia reticulata (Saarikoski & Viluksela 1982)

1844 • 1,1,1,2-Tetrachloroethane 630-20-6

Synonyms	s-Tetrachloroethane
Sumformula of the chemical	C2H2Cl4
Use	Used as a solvent and in the manufacture of a number of widely used products.
State and appearance	Liquid will sink and slowly dissolve.
Molecular weight	167.83
Specific gravity (water=1)	1.5532 20 °C
Water solubility, mg/l	2850 25 °C
Melting point, °C	-68.1
Boiling point, °C	129
Log octanol/water coefficient, log Pow	2.66
Other physicochemical properties	Container may explode in heat of fire.
Photochemical degradation in air	The photo oxidative reactivity of 1,1,1,2-tetrachloroethane is three times less than that of the 1,1,2,2-isomer. Irradiation of 10 ppm 1,1,1,2-tetrachloroethane in dry air in the presence of 4 ppm chlorine for 3 minutes consumed 2.0 ppm or the chlorinated ethane to give 4.0 ppm HCl, 1.5 ppm phosgene, 1.0 ppm formyl chloride, 1.0 ppm CO, 0.2 ppm trichloroacetyl chloride, and 0.1 ppm CO2 (Sax 1986).
Metabolism in mammals	A study of the metabolism of 1,1,1,2-tetrachloroethane in rats and guinea pigs given oral doses indicate the solvent is metabolized to trichloroethanol and excreted in the urine as trichloroethyl-.β.-d-glucuronic acid. In rats small amounts of trichloroacetic acid were also formed (Sax 1986).

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Bioconcentration factor, other organisms	14.4	estimated, edible portion of aquatic organisms consumed by Americans (Sax 1986)
Other information about bioaccumulation	Chlorinated ethanes exhibit greater bioconcentrating potential with increased chlorination. Bioconcentration factor in bluegill ranged from 2 for the 1,2-isomer to 140 for hexachloroethane (Sax 1986).	
TDLo values to mammals in oral exposure, mg/kg	129000	orl-mus, 2Y-I, tumorigenic (Sax 1986)
Health effects	Contact may cause burns to skin and eyes. Symptoms of exposure: albuminuria, CNS depressant, coma, conjunctivitis, dermatitis, dizziness, hematuria, hepatomegaly, jaundice, nausea and vomiting, nephritis, oliguria, polyneuritis, somnolence, tremors, weight loss. May be fatal if inhaled, swallowed, or absorbed through skin (Sax 1986). Skin and eye irritation data: skn, rbt, 500 mg, 24hr; eye, rbt, 100 mg, severe (Sax 1986)	
Carcinogenicity	NCI carcinogenesis bioassay completed; result positive: mouse; results negative: rat (Sax 1986).	
Mutagenicity	Not mutagenic in Ames Salmonella assay. Mutagenic in rat (Sax 1986).	
LC50 values to crustaceans, mg/l	24	48hr, Daphnia magna (LeBlanc 1980)
	23.9 27	48hr, Daphnia magna 24hr, Daphnia magna (Sax 1986)
LC50 values to fishes, mg/l	20	96hr, Lepomis macrochirus (Buccafusco et al. 1981)
	19.6 20	96hr, Lepomis macrochirus 24hr, 96hr, Lepomis macrochirus, young (Sax 1986)

1845 • 1,1,2,2-Tetrachloroethane 79-34-5

Synonyms	Acetylenetetrachloride	
Sumformula of the chemical	$C_2H_2Cl_4$	
Use	Manufacturing of 1,1-dichloroethylene; solvent for chlorinated rubber and other organic materials; bleach manufacturing. Intermediate; byproduct.	
State and appearance	Colourless liquid.	
Molecular weight	167.84	
Vapour pressure, mmHg	5	20 °C
Water solubility, mg/l	2900 3000 3200 > 1000 mg/l	20 °C 25 °C (Dilling 1977) 25 °C (Neely et al. 1974) (MITI 1992)
Melting point, °C	-42.5 – -43.8 -44	 (Suntio et al. 1988)
Boiling point, °C	146.3	(MITI 1992)
Log octanol/water coefficient, log Pow	2.39–3.01 2.45 2.39	(Sabljic 1987) (Anon. 1988) (Banerjee et al. 1980)

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Henry's law constant, Pa x m^3/mol	39 (Anon. 1988) 44.76 calc. (Suntio et al. 1988) 33.45 calc. (Yaws et al. 1991)
Volatilization	Relative volatility (nBuAc=1) = 0.65
Mobility	Equilibrium distribution: *mass %* air 92.75 water 6.95 solid 0.30 (Anon. 1988)
Total degradation in water	Biodegradation: 0% by TOC; period:28d; substance: 100 mg/l; sludge: 30 mg/l 10% by GC analysis; period: 28d; substance: 100 mg/l; sludge: 30 mg/l (MITI 1992)
Bioconcentration factor, fish	7 32d, Pimephales promelas (USEPA 1984) 4.5–13.2 6w, Cyprinus carpio, conc 0.26 mg/l 4.1–13.1 6w, Cyprinus carpio, conc 0.026 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	800 orl-rat (Lewis & Sweet 1984)
LDLo values to mammals in oral exposure, mg/kg	300 orl-dog (Lewis & Sweet 1984)
LCLo values to mammals in inhalation exposure, ppm	1000 4hr, ihl-rat (Lewis & Sweet 1984)
TDLo values to mammals in oral exposure, mg/kg	30 orl-hmn (Lewis & Sweet 1984)
Carcinogenicity	NCI carcinogenesis bioassay completed: results positive, mus; results indefinite, rat (Lewis & Sweet 1984).
LC50 values to crustaceans, mg/l	9.3 48hr, Daphnia magna (LeBlanc 1980) 62.1 48hr, unfed, Daphnia magna, 56.9 48hr, fed, Daphnia magna (USEPA 1984)
EC50 values to crustaceans, mg/l	23 48hr, unfed, Daphnia magna 25.2 48hr, fed, Daphnia magna (USEPA 1984)
NOEC values to crustaceans, mg/l	6.85–14.4 28d, Daphnia (USEPA 1984)
LC50 values to fishes, mg/l	12 96hr, Cyprinodon variagetus (Heitmuller et al. 1981) 37 7d, Poecilia reticulata (Könemann 1979) 20.3 96hr, Pimephales promelas (Veith et al. 1983) 21 96hr, Lepomis macrochirus (Buccafusco et al. 1981) 20.4 96hr, flow-through, Pimephales promelas (USEPA 1984) 31 48hr, Oryzias latipes (MITI 1992)
NOEC values to fishes, mg/l	1.4–4.0 32d, Pimephales promelas (USEPA 1984)

1846 • Tetrachloroethylene

127-18-4

Synonyms	1,1,2,2-Tetrachloroethylene Perchloroethylene Tetrachloroethene Perchloroethene	
Sumformula of the chemical	C_2Cl_4	
Use	Dry clearing solvent; metal degreasing; solvent for fats, greases, waxes; remove soot from industrial boilers; intermediate; vapour degreasing solvent; drying agent for metals and certain other solids; vermifuge, heat transfer medium, manufacture of fluorocarbons.	
State and appearance	Colourless liquid.	
Odour	Ether-like odour.	
Molecular weight	165.82	
Density, kg/m³	1623	20 °C
Vapour pressure, mmHg	14 18.49 18.47	20 °C 25 °C (Daubert & Danner 1985) 25 °C (Riddick et al. 1986)
Water solubility, mg/l	150.3 150 < 10 000	25 °C (Horvath 1982) 20 °C (Anon. 1986b) (MITI 1992)
Melting point, °C	-19 -19	(Suntio et al. 1988) (MITI 1992)
Boiling point, °C	121 121.2	(Anon. 1986b) (MITI 1992)
Log octanol/water coefficient, log Pow	2.53–2.88 2.53 3.38 2.6 2.88 2.6 2.53 2.88 3.4	(Sabljic 1987) (Anon. 1986b) (Anon. 1988) (Schwarzenbach & Westall 1981) (Schwarzenbach et al. 1983) (Chiou et al. 1977) (Banerjee et al. 1980) (Neely et al. 1974) (Hansch & Leo 1985)
Log organic C/water coefficient, log Pcw	2.32 2.36	exptl (Schwarzenbach & Westall 1981) calcd (Schwarzenbach & Westall 1981)
Henry's law constant, Pa x m³/mol	730 1793 2720	(Anon. 1988) exptl. (Gossett 1987) calc. (Yaws et al. 1991)
Volatilization	Relative volatility (nBuAc=1) = 1.95 PCE will evaporate rapidly from water based on estimates of half-life for the evaporation from water which range from fractions of an hour to several hours in laboratory experiments. Due to its high vapour pressure and low adsorption to soil, volatilization of PCE from dry soil should be rapid. (Howard1990)	
Adsorption/desorption	When PCE adsorbed to silica gel is irradiated through a pyrex filter, 60–90% is lost in 6 days. (Gaeb et al. 1977)	

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Mobility	Equilibrium distribution: *mass %* air 99.45 water 0.40 solid 0.15 (Anon. 1988). Theoretical distribution: > 99% in air, < 0.2 in water (Anon. 1989). Koc: 209 (Schwarzenbach 1981) 210 (Chiou et al. 1979) A Koc of 238 was calculated based on a reported Kom of 137.7 in a peaty soil. (Lyman et al. 1982) (Fresenius 1984) Based on reported and estimated Koc's, PCE will be expected to exhibit low to medium mobility in soil (Swann et al. 1983) Extremely stable, resist hydrolysis. Insoluble in water (Sax & Lewis 1987).
Photochemical degradation in air	PCE reacts with hydroxyl radicals which are produced by sunlight in the troposphere with an estimated half-life of about 2 months or a loss of 1.5% per sunlit day. (Howard 1990) Photooxidation in pure air with simulated tropospheric light is with complete degradation occurring in 7 days and from 0.5% to 100% loss per hour. The rate of loss is very sensitive to radiation in the 280–330 nm region and increases with increasing PCE concentration. The presence of nitrogen oxides has little effect on the rate of loss, and the main reaction product is phosgene (70–85%) with smaller amounts of carbon tetrachloride (8%), dichloroacetyl chloride and trichloroacetyl chloride. The proposed mechanism involved the molecular reaction with chlorine radicals produced by photooxidation of PCE. (Singh et al. 1975; Dimitriades et al. 1983) Some photodegradation occurs when PCE in air-saturated water is exposed to sunlight. In one year, 75% degradation occured whereas 59–65% degradation was noted for dark controls. (Dilling et al. 1975)
Other reactions in atmosphere	Hydroxyl radicals in troposphere (half-life 100 days) can attack double bonds when intermediate products are formed which propably are then hydrolyzed to trichloroacetic acid (Pearson & McConnell 1975).
Photochemical degradation in water	No photochemical degradation in water (Rippen 1988).
Hydrolysis in water	Hydrolysis in aerobic conditions, half-life > 9 months (Rippen 1988).
Aerobic degradation in water	Surface, no measurable degradation in 6 weeks (Hellmann 1985).
Total degradation in water	If PCE is released in water, the primary loss will be by evaporation. The half-life for evaporation from water will depend on wind and mixing conditions and is estimated to range from 3 hours to 14 days in rivers, lakes and ponds. Chemical and biological degradation are expected to be very slow. PCE will not be expected to significantly bioconcentrate in aquatic organisms or to adsorb to sediment. (Howard 1990) In a seawater aquarium, an 8-day half-life was demonstrated to be predominately the result of evaporation. (Jensen & Rosenberg 1975) In a natural pond PCE disappeared in 5 and 36 days at low (25 ppm) and high (250 ppm) dose levels, respectively. (Lay et al. 1984) Biodegradation: 11% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992)
Degradation and transformation products	Trichloroethene, dichloroethene and vinylchloride after anaerobic degradation (Anon. 1989).

Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Other information about degradation	Degradation of tetrachloroethylene:

ENVIRONMENT	*INIT.CONC. mg/l*	*REDOX-COND.*	*TEMP. °C*	*DEGRADATION %/day*	*t1/2*	*REF.*
biofilm	0.015	methanogen	22	–	87 (1)	a
water + soil	0.085–0.666	anaerobic	20	< 5/7		b
water	0.010	methanogen	35	30/112	218	c
water	0.032	methanogen	35	38/112	165	c
water	0.130	methanogen	35	57/112	92	c
water	0.0088	aerobic	20	0/175		c
water	0.033	aerobic	20	0/175		c
water	0.074	aerobic	20	0/175		c
biofilm	0.01	aerobic	22	0/730		d
water	0.152	methanogen	35	100/57	< 19	e
biofilm	0.170	methanogen	23	–	74 (1)	f
water (deion.)	1.0	aerobic	25	–	264	g
water	0.2	aerobic + methane	20	0/4		h
soil column	0.7	aerobic + methane	–	–	0.26	i
water	0.13	aerobic	–	97/11		j
soil	0.0878	aerobic/anaer.	25	67/21	12.7	k
soil	1.43	aerobic/anaer.	25	68/21	13.0	k
soil	0.25	aerobic/anaer.	25	15/11	46.2	k
water	5	aerobic	25	45/7		l
water	10	aerobic	25	30/7		l
water (adapted)	5	aerobic	25	87/7		l
water (adapted)	10	aerobic	25	84/7		l
water + soil	0.6–0.8	aerobic	17	< 2/7		m

(1) Biomass concentration set to 0.100 mg/l.

a) Bouwer & McCarty 1985
b) Wilson et al. 1983
c) Bouwer et al. 1981
d) Bouwer & McCarty 1982
e) Bouwer & McCarty 1983a
f) Bouwer & Wright 1987
g) Dilling et al. 1975
h) Fogel et al. 1986
i) Anon. 1987b
j) Kästner 1986
k) Parsons et al. 1984
l) Tabak et al. 1981
m) Wilson et al. 1983a
n) Vogel & McCarty 1985

No degradation occurred in 21 days in 3 biodegradability tests acclimated or un acclimated inocula or in a river die-away test. (Mudder 1982)

Metabolism in mammals	Quick uptake via skin and lungs. 70–90% of the uptaken amount is eliminated unchanged with exhale. Is metabolized mostly to trichloroacetic acid which is excreted in urine (Fawell & Hunt 1988).
Bioconcentration factor, fishes	39 — Salmo gairdneri (Verschueren 1983) 49 — 21d, Lepomis macrochirus (Davies & Dobbs 1984) 74 — 32d, Pimephales promelas (USEPA 1984) 38.9 — Pimephales promelas (Neely et al. 1974) 49 — Lepomis macrochirus (Barrows et al. 1980) 25.8–77.1 — 8w, Cyprinus carpio, conc 0.1 mg/l 28.4–75.7 — 8w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).

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LD50 values to mammals in oral exposure, mg/kg	8850 orl-rat 8100 orl-mus (Lewis & Sweet 1984) 2600 orl-rat (Torkelson & Rowe 1982)
LC50 values to mammals in inhalation exposure, mg/m³	27800 6hr, ihl-rat (Bonnet et al. 1980)
LDLo values to mammals in oral exposure, mg/kg	4000 orl-dog (NIOSH 1979)
LCLo values to mammals in inhalation exposure, ppm	4000 4hr, ihl-rat (Lewis & Sweet 1984)
TCLo values to mammals in inhalation exposure, ppm	96 7hr, ihl-hmn (Lewis & Sweet 1984)
Other information about mammals	Maximum tolerable oral dose in 78 weeks was 720–1070 mg/kg/d for mouse and rat (NCI 1977).
Health effects	Irritant to eyes and skin (Sax & Lewis 1987).
Carcinogenicity	NCI carcinogenesis bioassay completed: results positive, mus; results negative, rat (Lewis & Sweet 1984).
Mutagenicity	Positive in Ames test (IARC 1979). Negative in chromosome aberration test (IARC 1979). Restricted evidence of carcinogenicity in mice (IARC 1979).
Teratogenicity	Teratogenic effects have not been proved but there have been some toxic effects to fetuses (Fawell & Hunt 1988).
Maximum longterm immission concentration in air for plants, mg/m³	35 VDI 2306
Maximum longterm immission concentration in air for plants, ppm	5 VDI 2306
Effects on microorganisms	EC10, Pseudomonas putida, 51 mg/l, 16hr, pH 7 (Anon. 1986b)
Effects on wastewater treatment	Inhibition in active sludge 10 mg/l (Neumann 1984).
EC50 values to algae, mg/l	> 816 mg/l 96hr, Selanastrum capricorntum, chlorophyll a > 816 mg/l 96hr, Selanastrum capricorntum, cellnumber (Anon. 1986b) 10.5 Phaeodactylum (Pearson & McConnell 1975)
LOEC values to algae, mg/l	2 phytoplankton, flow through (Erickson & Hawkins 1980)
LC50 values to crustaceans, mg/l	17.7 48hr, Daphnia magna (Anon. 1986b) 30.84 Tanytarsus dissimilis (Anon. 1986b) 18.1 48hr, unfed, Daphnia magna 9.09 48hr, fed, Daphnia magna (USEPA 1984) 10 96hr, Mysidopsis (Zaroogian et al. 1985)
EC50 values to crustaceans, mg/l	147 24hr, Daphnia magna (Anon. 1986b) 8.5 48hr, unfed, Daphnia magna 7.49 48hr, fed, Daphnia magna (USEPA 1984) 18 48hr, Daphnia magna (LeBlanc 1980)
NOEC values to crustaceans, mg/l	0.505–1.11 28d, Daphnia (USEPA 1984)

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LC50 values to fishes, mg/l	4.99	96hr, Salmo gairdneri (Shubat et al. 1982)
	13	96hr, Lepomis macrochirus (Buccafusco et al. 1981)
	18.4	96hr, Pimephales promelas
	18	96hr, Salmo gairdneri (Alexander et al. 1978)
	24	96hr, Pimephales promelas (Broderius & Kahl 1985)
	130	48hr, Leuciscus idus melanotus
	18.4	96hr, Pimephales promelas
	13.46	Pimephales promelas
	21.4	96hr, Pimephales promelas
	12.9	Lepomis macrochirus
	7	96hr, Lepomis macrochirus
	4.8	Salmo gairdneri
	5.8	Salmo gairdneri (Anon. 1986b)
	13.4	96hr, Pimephales promelas
	4.99	96hr, Salmo gairdneri
	5.76	96hr, a mixture with dimethylforamide Salmo gairdneri (USEPA 1984)
	5	96hr, Limanda, sea water, flow trough (Pearson & McConnell 1975)
	32	48hr, Oryzias latipes (MITI 1992)
EC50 values to fishes, mg/l	4.86	96hr, Salmo gairdneri, USEPA 1984
	5.84	96hr, a mixture with dimethylforamide Salmo gairdneri (USEPA 1984)
NOEC values to fishes, mg/l	0.5–1.4	32d, Pimephales promelas (USEPA 1984)
Effects on the physiology of water organisms	Poecilia sphenops, 60 days, 17% survival, decreased weight and injuries in liver, 1.6 mg/l (Loekle et al. 1983).	
Effects on the reproduction of water organisms	Daphnia, growth, reproduction, 28 days, EC0, 0.5–1.1 mg/l (Rippen 1988). Pimephales, embryo, larvae, 32 days, EC0, 0.5–1,4 mg/l (Rippen 1988).	
Other information about water organisms	EC50 (24hr) 100 mg/l, rpd, Tetrahymena pyriformis (Yoshioka et al. 1985). LC50, Dugesia (Planarie), 25 mg/l (Yoshioka et al. 1986). LC50 (48hr), Elminius, 3,5 mg/l (Pearson & McConnell 1975).	
Other information	Estimated amount in troposphere: 0.7 Mt (1980) which is 3.3% of the total amount of organic bound chlorine (Fabian 1986).	

1847 • Tetrachloroguaiacol 2539-17-5

Synonyms	2-Methoxytetrachlorophenol 3,4,5,6-Tetrachloroguaiacol
Sumformula of the chemical	C7H4O2Cl4
Use	Chlorinated guaiacols are formed by the reaction of chlorination agents during the bleaching process.
Molecular weight	261.91
Melting point, °C	122–124
pKa	6.25
Log octanol/water coefficient, log Pow	4.31 4.605 (Xie et al. 1984)

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Mobility	1.37% (air), 27.06% (water), 71.58% (sediment)	
LD50 values to mammals in oral exposure, mg/kg	1690	orl-rat (Lewis & Sweet 1984)
LC50 values to fishes, mg/l	1.7 0.32 0.34	hrd (280 mgCaCO3/l), pH 7.3–8.1, 96hr sfd (6 mgCaCO3/l), pH 6.4, 96hr hrd (280 mgCaCO3/l), pH 6.4–7.0, 96hr Salmo gairdneri (Voss et al. 1980)
	0.32	96hr, Salmo gairdneri (Leach & Thakore 1975)
	0.11	4d, Alburnus alburnus (Oikari 1987)

1848 • 2,3,4,5-Tetrachloronitrobenzene 879-39-0

EC50 values to microorganism, mg/l	3.2	Microtox (Kaiser and Ribo 1985)

1849 • 2,3,5,6-Tetrachloronitrobenzene 117-18-0

EC50 values to microorganism, mg/l	6.5	Microtox (Kaiser and Ribo 1985)

1850 • 2,3,4,5-Tetrachlorophenol 4901-51-3

Sumformula of the chemical	C6H2OCl4	
Molecular weight	231.88	
Melting point, °C	95–98 116–117 °C	 (Suntio et al. 1988)
pKa	6.96 5.64	
Log octanol/water coefficient, log Pow	4.42–4.87 5.03 5.03	(Sabljic 1987) (Geyer et al. 1987) (Banerjee et al. 1984)
Log soil sorption coefficient, log Kom	4.12 3.32	observed (Sabljic 1987) calculated (Sabljic 1987)
Aerobic degradation in soil	AEROBIC DEGRADATION IN SOIL Maximum adsorption wavelength: 300 nm NON-STERILE SOIL % decomposition at the termination of the experiment: 160d, 31% STERILE SOIL % decomposition at the termination of the experiment: 160d, -1% (Baker et al. 1980)	
Anaerobic degradation in soil	ANAEROBIC DEGRADATION IN SOIL Maximum adsorption wavelength: 300 nm NON-STERILE SOIL % decomposition at the termination of the experiment: 80d, 5% STERILE SOIL % decomposition at the termination of the experiment: 80d, 7% (Baker et al. 1980)	

Other information about degradation	Degradation of 2,3,4,5-tetrachlorophenol:

ENVIRONMENT	INIT.CONC. mg/l	REDOX-COND.	TEMP. °C	DEGRADATION %day	REF.
water (PCP-ad.)	–	aerobic	–	44/1	a
soil	1	aerobic	23	31/160	b
sterile soil	1	aerobic	23	1/160	b
soil	1	anaerobic	23	5/80	b
sterile soil	1	anaerobic	23	7/80	b
soil	100	anaerobic	28	68/28	c

a) Steiert & Crawford 1985 b) Baker & Mayfield 1980
c) Ide et al. 1972 (Anon. 1987b).

LD50 values to mammals in oral exposure, mg/kg	400	orl-mus (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	97	ipr-mus (Lewis & Sweet 1984)
LC50 values to fishes, mg/l	< 0.5	96hr, Salmo gairdneri (Voss et al. 1980)
	0.44	96hr, Pimephales promelas (Holcombe et al. 1984)
	0.77	96hr, Poecilia reticulata (Könemann 1979)
	0.205	96hr, Salmo gairdneri (Holcombe et al. 1984)

1851 • 2,3,4,6-Tetrachlorophenol 58-90-2

Sumformula of the chemical	C6H2OCl4	
Use	Fungicide.	
State and appearance	Needles.	
Molecular weight	231.88	
Vapour pressure, mmHg	60	190 °C
Water solubility, mg/l	100	25 °C (Mabey et al. 1982)
	183	25 °C, pH 5.1 (Blackman et al. 1955)
	23	(MITI 1992)
Melting point, °C	69–70	(Suntio et al. 1988, MITI 1992)
Boiling point, °C	164	23 mmHg (MITI 1992)
pKa	5.38	
	5.22	
Log octanol/water coefficient, log Pow	4.38	(Xie 1984)
	4.1	(Hansch & Leo 1979)
Log soil sorption coefficient, log Kom	3.35	observed (Sabljic 1987)
	3.32	calculated (Sabljic 1987)
Henry's law constant, Pa x m³/mol	0.2337	calc. (Suntio et al. 1988)
Total degradation in soil	Biodegradation: decomposition in soil suspensions: > 72 days for complete disappearance (Verschueren 1983).	
Total degradation in water	Biodegradation: 7% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992)	

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Other information about degradation	Degradation of 2,3,4,6-tetrachlorophenol: *ENVIRONMENT* / *INIT.CONC. mg/l* / *REDOX-COND.* / *TEMP. °C* / *DEGRADATION %/day* / *REF.* water (PCP-ad.) / – / aerobic / – / 100/1 / a soil suspension / 10–100 / aerobic / 30 / 100/72 / b soil / 100 / anaerobic / 28 / 68/28 / c a) Steiert & Crawford 1985 b) Alexander & Aleem 1961 c) Ide et al. 1972 (Anon. 1987b).
Bioconcentration factor, fishes	93 Carassius auratus (Verschueren 1983) 25–6 8w, Cyprinus carpio, conc 0.01 mg/l 36–95 8w, Cyprinus carpio, conc 0.001 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	140 orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	250 skn-rbt (Lewis & Sweet 1984)
LC50 values to crustaceans, mg/l	0.29 48hr, Daphnia magna (LeBlanc 1980)
LC50 values to fishes, mg/l	0.14 96hr, Lepomis macrochirus (Buccafusco et al. 1981) 0.75 24hr, Carassius auratus (Kobayashi 1979) 1.1 48hr, Oryzias latipes (MITI 1992)

1852 • 2,3,5,6-Tetrachlorophenol 935-95-5

Molecular weight	231.88
Melting point, °C	114–116
Other information about degradation	Degradation of 2,3,5,6-tetrachlorophenol: *ENVIRONMENT* / *INIT. mg/l* / *REDOX COND.* / *TEMP. °C* / *DEGRADATION %/day* / *REF.* water (PCP-ad.) / - / aerobic / - / 100/1 / a soil / 100 / anaerob. / 28 / 94/28 / b a) Steiert & Crawford 1985 b) Ide et al. 1972 (Anon. 1987b).
LD50 values to mammals in oral exposure, mg/kg	109 orl-mus (Lewis & Sweet 1984)
LC50 values to crustaceans, mg/l	0.57 49hr, Daphnia magna (LeBlanc 1980)
LC50 values to fishes, mg/l	0.17 96hr, Lepomis macrochirus (Buccafusco et al. 1981) 1.37 24hr, Poecilia reticulata (Könemann 1979) 1.9 96hr, Cyprinodon variegarus (Heitmuller et al. 1981)
Other information about water organisms	Tetrahymena pyriformis, 1.01 mg/l, 2 d, EC50, grw (Schultz 1987).

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1853 • Tetrachlorophthalic acid monoamide 56113-42-9

Sumformula of the chemical	C8H3O3NCl4	
Water solubility, mg/l	14000	(MITI 1992)
Log octanol/water coefficient, log Pow	-1.68	(MITI 1992)
Bioconcentration factor, fishes	< 0.3 < 3.1	6w, Cyprinus carpio, conc 0.5 mg/l 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 500	48hr, Oryzias latipes (MITI 1992)

1854 • Tetrachlorophthalimide 1571-13-7

Sumformula of the chemical	C9HO2Cl4N	
Water solubility, mg/l	< 10	(MITI 1992)
Total degradation in water	Biodegradation: 0–1% by BOD (hydrolysed to Tetrachlorophthalic acid monoamide) period: 28 d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	

1855 • 1,2,2,3-Tetrachloropropane 13116-53-5

Sumformula of the chemical	C3H4Cl4	
Water solubility, mg/l	480	(MITI 1992)
Log octanol/water coefficient, log Pow	2.72	(MITI 1992)
Total degradation in water	Biodegradation: 1% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	12–54 22–52	8w, Cyprinus carpio, conc 0.2 mg/l 8w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	35.43	48hr, Oryzias latipes (MITI 1992)

1856 • Tetraethyl lead 78-00-2

Synonyms	TEL Lead tetraethyl Tetraethylplumbane
Sumformula of the chemical	C8H20Pb

Purity, %	100
Use	Anti-knock compounds for gasoline. TEL has been largely replaced by MBTE.
State and appearance	Colourless oily liquid.
Odour	Pleasant characteristic odour.
Molecular weight	323.47
Specific gravity (water=1)	1.659
Density, kg/m³	1659
Vapour pressure, mmHg	0.47 20 °C 2.5 55 °C 19 91 °C
Water solubility, mg/l	0.8 20 °C 30 25 °C
Melting point, °C	-136.8
Boiling point, °C	198
Degradation point, °C	110–200 °C
Flashing point, °C	85
Log octanol/water coefficient, log Pow	3
Other physicochemical properties	In dilute solution in water decomposes to give triethyl salt, then diethyl salt and finally inorganic lead (Verschueren 1983). Soluble in all organic solvents, insoluble in water and dilute acids or alkalies. Decomposes slowly at room temperature, rapidly at 125–150 °C (Sax & Lewis 1987).
Other reactions in atmosphere	Degradation in summertime: 88% in hour (Harrison & Laxen 1978).
Photochemical degradation in soil	Photochemical degradation to toxic trialkyl lead (Ter Haar & Bayard 1971).
Other chemical degradation processes	In combustion of alkyl lead unstable relatively soluble lead haloginades are formed. The end products in exhaust fumes are lead carbonate, lead oxides and leadoxycarbonate (Ter Haar & Bayard 1971).
Other information about degradation	Sunlight decomposes to toxic triethyl lead. Lead in any salt form is a hazard (Sax 1986). Degradation in summer time: 88% in hour (Harrison & Laxen 1986).
Other information about metabolism	Food chain contamination potential: Both fish and animals are capable of accumulationg lead and passing it on. Positive (Sax 1986). Tetraalkyl lead is metabolized to toxic trialkyl lead which gradually is metabolized to inorganic lead (Oskarsson & Camner 1983). Half-life in rat; in heart, 7 days; in blood, 3–4 days (Hayakawa 1972). The difference in lead metabolia between species is markable (Granjean & Nielsen 1979).
Bioconcentration factor, fishes	130 96hr, Pleuronectes platessa (Verschueren 1983)
Bioconcentration factor, mollusca	120 Mytilus, 96hr (Verschueren 1983)
Bioconcentration factor, crustaceans	650 crayfish (Verschueren 1983)

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Other information about bioaccumulation	Potential for bioaccumulation: lead accumulates in bones. Positive; a lipoid solvent (Sax 1986).	
LD50 values to mammals in oral exposure, mg/kg	12.3	orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	15	par-rat (Sax 1986)
LC50 values to mammals in inhalation exposure, mg/m³	850	60 min, ihl-rat (Lewis & Sweet 1984)
LDLo values to mammals in oral exposure, mg/kg	17 30	orl-rat orl-rbt (Sax 1986)
LDLo values to mammals in non-oral exposure, mg/kg	547	skn-dog (Lewis & Sweet 1984)
	10 31 86 830 32 23 995	ipr-rat ivn-rat scu-mus skn-rbt scu-rbt ivn-rbt skn-gpg (Sax 1986)
LCLo values to mammals in inhalation exposure, mg/kg	650	7hr, ihl-mus (Sax 1986)
TDLo values to mammals in oral exposure, mg/kg	11 7.5 11	orl-rat, 6-16d preg, teratogenic orl-rat, 12-14d preg, teratogenic orl-mus, 5-15d preg, teratogenic (Sax 1986)
TDLo values to mammals in non-oral exposure, mg/kg	100	scu-mus, 21D-I, tumorigenic (Sax 1986)
Health effects	May be absorbed via skin. Highly toxic by all routes. Emits toxic fumes when heated. An accumulative poison (Sax 1986).	
Effects on wastewater treatment	May plug filters and exchange beds (Sax 1986). Will sink rapidly and dissolve very slowly (Sax 1986).	
EC50 values to algae, mg/l	< 0.3	pht, 4hr, Ankistrodesmus falcatus (Silverberg et al. 1977)
	0.15	48hr, Dunaliella (Marchetti 1978)
LC50 values to crustaceans, mg/l	0.02	96hr, crayfish (Maddock & Taylor 1977)
	0.085	48hr, Artemia, nauphids (Marchetti 1978)
LC50 values to fishes, mg/l	0.02	96hr, Lepomis macrochirus (Verschueren 1983)
	0.065	48hr, Morone labrox (Marchetti 1978)
	0.2	96hr, Lepomis macrochirus (Jones 1971)
	0.23	96hr, Pleuronectes (Maddock & Taylor 1977)
Effects on the physiology of water organisms	Poteriochromonas malhamensis, 0.200 mM, EC50, phy, 0.13d (Roderer 1986).	
Other information about water organisms	LC50, 96hr, Mytilus, 0.10 mg/l (Maddock & Taylor 1977).	
Other information	Air pollution high (Sax 1986).	

1857 • Tetraethyl tin

597-64-8

EC50 values to algae, mg/l	0.142	72hr, rpd, Skeletonema costatum (Walsh et al. 1985)

1858 • Tetraethylpyrophosphate 107-49-3

Synonyms	TEPP Ethyl pyrophosphate Diphosphoric acid, tetraethyl ester Pyrophosphoric acid, tetraethyl ester
Sumformula of the chemical	C8H2007P2
Use	Insecticide, rodenticide.
State and appearance	White to amber liquid.
Molecular weight	290.22
Specific gravity (water=1)	1.185
Vapour pressure, mmHg	0.000155 20 °C
Boiling point, °C	135–138
Degradation point, °C	thermal decomposition range 170-213 °C with formation of ethylene (Sax 1986)
Other physicochemical properties	Flammable. Toxic combustion products: Vapours of unburned material and phosphoric acid emitted. Soluble in water. Will hydrolyse. Water solution attacks metals.
Hydrolysis in water	Rapidly hydrolysed by water, half-life 6.8hr (pH 7, 25 °C) (Verschueren 1983)
Total degradation in soil	Decomposes rapidly in presence of moisture, usually within 48hr (Sax 1986).
Total degradation in water	Forms phosphoric acid and ethylene gas. Material will hydrolyse quickly; half-life at 25 °C approximately 7hr in a 50 v/v mixture.– Will give acid solution. Will also be corrosive to metals.
Other information about degradation	Nonpersistent. Readily hydrolysed, therefore are not persistent in soils and water (Sax 1986).
Other information about bioaccumulation	Organophosphates are highly toxic to birds, mammals, and fish and would kill the organism before it would be taken into the tissues. Even when these chemicals are taken up by fish, they seldom persist for longer than a week (Sax 1986).
LD50 values to mammals in oral exposure, mg/kg	0.5 orl-rat 1.2 orl-mam 7 orl-mus (Lewis & Sweet 1984) 1.05 orl-rat 2.3 orl-gpg (Sax 1986)
LD50 values to mammals in non-oral exposure, mg/kg	2.4 skn-rat (Lewis & Sweet 1984) 0.85 ipr-rat 1 scu-mus 5 skn-rbt 0.65 ipr-rat 0.3 ivn-rat 1.8 ims-rat 0.83 ipr-mus 0.52 scu-mus 0.2 ivn-mus (Sax 1986)
LDLo values to mammals in oral exposure, mg/kg	2 orl-hmn (Sax 1986)
LDLo values to mammals in non-oral exposure, mg/kg	0.4 ims-hmn (Sax 1986)

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TDLo values to mammals in oral exposure, mg/kg	0.432	orl-hmn (Lewis & Sweet 1984)
TDLo values to mammals in non-oral exposure, mg/kg	0.1	par-hmn (Sax 1986)
Other information about mammals	ALD = 1.6–3.7 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987).	
Health effects	Direct contact: Material will be absorbed quickly through the skin. It will irritate skin and eyes. General sensation: Acute poisoning from inhalation or skin absorption produces headaches, weakness, dizziness, anxiety, tremors of the tongue and eyelids, and impairment of visual acuity. Prolonged contact may result in salivation, tearing, abdominal cramps, vomiting, sweating, and muscular fasciculations. Death may occur from respiratory difficulty, cyanosis, and convulsions. – Material is a choliesterase inhibitor. Highly toxic through inhalation and skin absorption. Small doses at frequent intervals are largely additive (Sax 1986).	
LD50 values to birds in oral exposure, mg/kg	3.56 1	orl-dck orl-bwd (Lewis & Sweet 1984)
LD50 values to birds in dermal exposure, mg/kg	64 0.18	skn-dck (Lewis & Sweet 1984) ivn-pgn (Sax 1986)
Effects on amphibia	LD50, 540 mg/kg, par, frog (Sax 1986).	
Effects on wastewater treatment	Not significantly degraded. Less than 5% of COD was utilized. Not amenable to biological treatment at a municipal sewage treatment plant (Sax 1986).	
LOEC values to algae, mg/l	10	10 d, Chlorella sp. Phaeodactylum tricornurum Monochrystis lutheri (Davis & Hidu 1969)
LC50 values to crustaceans, mg/l	0.039	96hr, Gammarus lacustris (Sanders 1969)
LC50 values to fishes, mg/l	1.9 1.1	96hr, Pimephales promelas 96hr, Lepomis macrochirus (Pickering et al. 1962)
Other information about water organisms	500 mg/l, marine plankton, no growth or lethal (Sax 1986). LC50, 48hr, > 10 mg/l, oyster larvae (Sax 1986).	
Other information	Air pollution: High-vapours are toxic when inhaled, and when heated it emits highly toxic fumes of phosphoric acid (Sax 1986).	

1859 • Tetrahydrofuran

109-99-9

Synonyms	THF	
Use	Solvent.	
Melting point, °C	-108.5	(MITI 1992)
Boiling point, °C	66	(MITI 1992)
Volatilization	Relative volatility (nBuAc=1) = 4.85	
Total degradation in water	Biodegradation: 100% by BOD period: 14d substance: 30 mg/l sludge: 30 mg/l (MITI 1992).	

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Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LDLo values to mammals in oral exposure, mg/kg	3000	orl-rat
LD50 values to birds in oral exposure, mg/kg	> 98	orl-Agelaius phoeniceus (Schafer et al. 1983)
Maximum longterm immission concentration in air for plants, mg/m³	30	VDI 2306
Maximum longterm immission concentration in air for plants, ppm	10	VDI 2306
LOEC values to algae, mg/l	225	rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)

1860 • Tetrahydrofurfuryl alcohol 97-99-4

LC50 values to fishes, mg/l	3400	48hr, Rasbora heteromorpha (Kemp et al. 1973)

1861 • Tetrahydronaphthalene 119-64-2

Synonyms	Naphthalene, 1,2,3,4-tetrahydro-	
Sumformula of the chemical	C10H12	
EINECS-number	2043402	
Boiling point, °C	200–209 (MITI 1992)	
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	118–237 147–536	8w, Cyprinus carpio, conc 0.38 mg/l 8w, Cyprinus carpio, conc 0.038 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	6.9	48hr, Oryzias latipes (MITI 1992)

1862 • cis-1,2,3,6-Tetrahydrophthalic acid anhydride 935-79-5

Sumformula of the chemical	C8H8O3	
Melting point, °C	102.2	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD (hydrolyzed to 4-Cyclohexene-1,2-dicarboxylic acid) period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

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1863 • Tetraisopropoxy titanate 546-68-9

Sumformula of the chemical	C12H2804Ti	
Melting point, °C	17	(MITI 1992)
Boiling point, °C	116	10 mmHg (MITI 1992)
Total degradation in water	Biodegration: 84–89% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

1864 • Tetralinhydroxyperoxide 771-29-9

EC50 values to algae, mg/l	0.7	72hr, rpd, Dunaliella bioculata (Heldal et al. 1984)

1865 • Tetramethyl lead 75-74-1

Synonyms	TML	
Sumformula of the chemical	(CH3)4Pb	
State and appearance	Colourless liquid.	
Density, kg/m³	1995	
Vapour pressure, mmHg	22.5	20 °C
Melting point, °C	-27.5	
Boiling point, °C	110	
Flashing point, °C	37.7	
Other physicochemical properties	Insoluble in water; slightly soluble in benzene, petroleum ether, alcohol; flammable, moderate fire risk (Sax & Lewis 1987).	
Photochemical degradation in air	Photochemical degradation to toxic trialkyl lead (Ter Haar & Bayard 1971).	
Other chemical degradation processes	In combustion of alkyl lead unstable relatively soluble lead halogenades are formed. The end products in exhaust fumes are lead carbonate, lead oxides and leadoxycarbonate (Ter Haar & Bayard 1971).	
Other information about degradation	Degradation in summertime: 21% in hour (Harrison & Laxen 1978).	
Other information about metabolism	Tetraalkyl lead is metabolized to toxic trialkyl lead which gradually is metabolized to inorganic lead (Oskarsson & Camner 1983). Differences in the metabolism of alkyl lead between species is markable (Grandjean & Nielsen 1979).	
Bioconcentration factor, fishes	60	96hr, Pleuronectes platessa (Grove)
Bioconcentration factor, mollusca	170	96hr, Mytilus (Grove)
Bioconcentration factor, crustaceans	20	crayfish, 96hr (Grove)
LD50 values to mammals in oral exposure, mg/kg	80–109	mg Pb/l, orl-rat (Cremer 1961)

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LC50 values to mammals in inhalation exposure, mg/m^3	> 9000	mg Pb/m^3, ihl-rat, 1hr (Henscler)
EC50 values to algae, mg/l	1.65	48hr, pht, Dunaliella terticulata (Marchetti 1978)
LC50 values to crustaceans, mg/l	0.25	48hr, Artemia salina (Marchetti 1978)
	0.11	Pb, 96hr, crayfish (Maddock & Taylor 1977)
LC50 values to fishes, mg/l	0.1	48hr, Morone labrax (Marchetti 1978)
	84	96hr, Lepomis macrochirus
	13.5	96hr, Menidia audens (TML 68% in toluene) (Dawson et al. 1977)

1866 • 1,2,3,4-Tetramethylbenzene 488-23-3

Sumformula of the chemical	C10H14	
Use	Solvent, plasticiser, intermediates.	
Molecular weight	134	
Log octanol/water coefficient, log Pow	3.98	(Anon. 1988)
	4	(Sangster 1989)
Henry's law constant, Pa x m^3/mol	440	(Anon. 1988)
Mobility	Equilibrium distribution:	
		mass %
	air	98.41
	water	0.64
	solid	0.95
		(Anon. 1988).

1867 • 1,2,4,5-Tetramethylbenzene 95-93-2

Sumformula of the chemical	C10H14	
Log octanol/water coefficient, log Pow	4.05	(Schwarzenbach & Westall 1981)
	4.1	(Sangster 1989)
Log soil sorption coefficient, log Kom	3.12	observed
	2.99	calculated (Sabljic 1987)
Henry's law constant, Pa x m^3/mol	2541 calc. (Yaws et al. 1991)	

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1868 • Tetramethylenedisulfoamine 80-12-6

Other information about mammals	ALD = 1.6 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987).

1869 • Tetramethylthiuram monosulfide 97-74-5

EC50 values to algae, mg/l	1	96hr, rpd, Chlorella pyrenoidosa (Leeuwen et al. 1985)
LC50 values to crustaceans, mg/l	2.9	48hr, Daphnia magna (Leeuwen et al. 1985)
LC50 values to fishes, mg/l	5.3	96hr, Poecilia reticulata (Leeuwen et al. 1985)

1870 • Tetrapropylenebenzenesulfonate 11067-81-5

Synonyms	Tetrapropylenebenzenesulfonic acid	
Effects on amphibia	NOEC, 3.2 mg/l, 100d, Xenopus laevis, mortality; NOEC, 10 mg/l, 100d, Xenopus laevis, development; NOEC, 10 mg/l, 100d, Xenopus laevis, growth (Slooff & Canton 1983).	
Effects on arthropods	NOEC, 10 mg/l, 25d, Culex pipiens, mortality; NOEC, 10 mg/l, 25d, Culex pipiens, development; (Slooff & Canton 1983).	
Effects on plants	NOEC, 1 mg/l, 7d, Lemna minor, specific growth rate (Slooff & Canton 1983).	
Effects on microorganisms	NOEC, 32 mg/l, 0,3d, Pseudomonas fluorescens, specific growth rate; NOEC, 32 mg/l, 4d, Microcystis aeruginosa, specific growth rate (Slooff & Canton 1983).	
NOEC values to algae, mg/l	1	4d, grw (biomass), Scenedesmus pannonicus (Slooff & Canton 1983)
LC50 values to crustaceans, mg/l	11	21d, Daphnia magna (van Leeuwen et al. 1987)
EC50 values to crustaceans, mg/l	4 8.3	48hr, rpd, Daphnia magna (Berglind & Dave 1984) Daphnia magna (van Leeuwen et al. 1987)
NOEC values to crustaceans, mg/l	10 3.2	21d, srv, Daphnia magna 21d, rpd, Daphnia magna (Slooff & Canton 1983)
LC50 values to fishes, mg/l	25	96hr, Gobius minutus (Adema 1976)
NOEC values to fishes, mg/l	10 10 10 3.2 3.2 10	28d, srv, Poecilia reticulata 28d, srv + bhv, Poecilia reticulata 28d, grw, Poecilia reticulata 40d, srv, Oryzias latipes 40d, srv + bhv, Oryzias latipes 40d, grw, Oryzias latipes (Slooff & Canton 1983)
Other information about water organisms	NOEC, 1 mg/l, 21d, Hydra oligactis, specific growth rate; NOEC, 3.2 mg/l, 40d, Lymnaea stagnalis, mortality; NOEC, 0.32 mg/l, 40d, Lymnaea stagnalis, reproduction; NOEC, 3.2 mg/l 40d, Lymnaea stagnalis, hatching (Slooff & Canton 1983).	
Other information	Toxicity decreases when the hardness of water increases (Berglind & Dave 1984).	

1871 • TFM 654-66-0

Synonyms	Sodium-4-nitro-3-trifluoromethylphenolate	
LC50 values to fish, mg/l	6.1 6	96hr, Salmo gairdneri 96hr, Salmo trutta m.lacustris (Dawson et al. 1977)

1872 • Thallium acetate 563-68-8

LC50 values to fishes, mg/l	170 31	96hr, Lepomis macrochirus 96hr, Menidia audens (Dawson et al. 1977)

1873 • Thallium and thallium compounds 7440-28-0

Molecular weight	204.37	
LDLo values to mammals in non-oral exposure, mg/kg	4.412	unk-man (Lewis & Sweet 1984)
TDLo values to mammals in oral exposure, mg/kg	5.714	orl-man (Lewis & Sweet 1984)
Effects on plants	Sunflower (Helianthus annuus) plants were kept in flasks containing solutions of heavy metal salts →photosynthesis was reduced by 50% of maximum when thallium concentrations of leaf tissue were 63 ppm (= 0.31 mM/g) (Bazzaz et al. 1974).	
LC50 values to crustaceans, mg/l	2.2	48hr, Daphnia magna (LeBlanc 1980)
LC50 values to fishes, mg/l	0.18	28d, Salmo gairdneri (Birge et al.1980)
LOEC values to fishes, mg/l	0.03	act, srv, Pimephales promelas (LeBlanc & Dean 1984)

1874 • Thallium sulfate 10031-59-1

Other information about mammals	ALD = 42.0 mg/l, act, orl, deer mouse (Virtanen & Nuuja 1987).

1875 • 1-(2-Thienyl)-2-nitroethene 874-84-0

Other information about mammals	LDfr = 43.3 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja1987).

1876 • Thiobencarb 28249-77-6

Use	Herbicide.	
Molecular weight	257.8	
LD50 values to mammals in oral exposure, mg/kg	1903 560	orl-rat orl-mus (Lewis & Sweet 1984)
LC50 values to algae, mg/l	0.29	rpd, 96hr, Skeletonema costatum (Borthwick & Walsh 1981)
LC50 values to crustaceans, mg/l	0.75	Daphnia pulex (Hashimoto & Nishiuchi 1981)
	0.37	96hr, Mysidopsis bahia (Borthwick & Walsh 1981)
LC50 values to fishes, mg/l	3.6 1.5	48hr, Carassius auratus 49hr, Cyprinus carpio (Hashimoto & Nishiuchi 1981)
	3.6	48hr, Cyprinus carpio (Pesticide Manual 1983)
	9.5	act, Sarotheredon aureus (Rao et al. 1983)

1877 • 4,4'-Thiobis(6-t-butyl-m-cresol) 96-69-5

Sumformula of the chemical	C22H30O2S	
EINECS-number	2025252	
Melting point, °C	162	(MITI 1992)

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Total degradation in water	Biodegradation: 1.9% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.12–4.2 6w, Cyprinus carpio, conc 0.3 mg/l < 1.3–11 Cyprinus carpio, conc 0.03 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	> 100 48hr, Oryzias latipes (MITI 1992)

1878 • 2,2'-Thiodiethanol 111-48-8

Synonyms	2,2'-Thiobis-ethanol
Sumformula of the chemical	C4H10O2S
EINECS-number	2038743
Melting point, °C	-16 (MITI 1992)
Boiling point, °C	168 14 mmHg (MITI 1992)
Total degradation in water	Biodegradation: 0–30% by BOD (on the upward trend) period: 28d substance: 100mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

1879 • Thioglycolic acid 68-11-1

Synonyms	Acetic acid, mercapto- Mercaptoacetic acid
Sumformula of the chemical	C2H4O2S
EINECS-number	2006774
Boiling point, °C	123 29 mmHg (MITI 1992)
Total degradation in water	Biodegradation: 100% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

1880 • Thiophanate-methyl 23564-05-8

Synonyms	Dimethyl-4,4'-(o-phenylene)bis(3-thioallophanate)
Sumformula of the chemical	C14H18N4O4S2

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Use	Active ingredient in fungicides.	
Molecular weight	342.42	
LD50 values to mammals in oral exposure, mg/kg	6640 3400 2270 3640	orl-rat orl-mus orl-rbt orl-gpg (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	1140 790	ipr-rat (Lewis & Sweet 1984) ipr-mus (Lewis & Sweet 1984)
LDLo values to mammals in oral exposure, mg/kg	4000	orl-dog (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	> 50000	orl-japonese qal (Verschueren 1983)
Effects on plants	Topsin-M was applied to soil using 70% a.i. wettable powder: 0.026 grams of Topsin-M available per plant caused decrease in chloroplast activity of the leaves of gherkin seedlings (van Wambeke et al. 1977).	
LC50 values to algae, mg/l	8.5	48hr, Chlorella pyrenoidesa (Canton 1976)
LC50 values to crustaceans, mg/l	16	48hr, Daphnia magna (Canton 1976)
LC50 values to fishes, mg/l	7.8 11	48hr, Salmo gairdneri (Canton 1976) 48hr, Cyprinus carpio (Pesticide Manual 1983)

1881 • Thiophene 110-02-1

Sumformula of the chemical	C4H4S	
EINECS-number	2037294	
Water solubility, mg/l	> 1000	(MITI 1992)
Melting point, °C	-37.1	(MITI 1992)
Boiling point, °C	84.4	(MITI 1992)
Log octanol/water coefficient, log Pow	1.86	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	1.8–3.2 < 7.2	6w, Cyprinus carpio, conc 0.15 mg/l 6w, Cyprinus carpio, conc 0.015 mg/l (MITI 1992)
LC50 values to fishes, mg/l	15.6	48hr, Oryzias latipes (MITI 1992)

1882 • Thiosemicarbazide 79-19-6

Other information about mammals	ALD = 94.0 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987).	
LD50 values to birds in oral exposure, mg/kg	9.10–11.0	orl-Sturnus vulgaris (Schafer et al. 1983)

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1883 • Thiourea

62-56-6

Melting point, °C	180	(MITI 1992)
Total degradation in water	Biodegradation: 2.6% by BOD substance: 30 mg/l sludge: 100 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.2 < 2	6w, Cyprinus carpio, conc 3 mg/l 6w, Cyprinus carpio, conc 0.3 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
EC50 values to microorganism, mg/l	3395	15 min Microtox (Govers et al. 1986)
LC50 values to fishes, mg/l	< 1000	48hr, Oryzias latipes (MITI 1992)

1884 • 9-Thioxanthone

492-22-8

Effects on arthropods	LC50, 1 d: Aedes aegypti, 0.0064 mg/l; Aedes taeniorhynchus, 0.540 mg/l; Culex quinquefasciatus, 2.82 mg/l (Borovsky et al. 1987).

1885 • Thiram

137-26-8

Synonyms	Tetramethylthiuram disulfide Bis(dimethylthiocarbamoyl)disuldide Tirama 50 *	
Sumformula of the chemical	C6H12N2S4	
Products containing the chemical	Tirama 50 * thiram 500 g/kg (PESREG)	
Use	Active ingredient in fungicides. Vulcanizing agent for rubber, especially for steam hose and other heat-resistant uses; insecticide; seed disinfectant; lube oil additive; bacteriostat; animal repellent.	
State and appearance	White, crystalline powder.	
Odour	Characteristic.	
Molecular weight	240.44	
Density, kg/m³	1420	
Vapour pressure, mmHg	0.0001	20 °C
Water solubility, mg/l	30	25 °C
Melting point, °C	155–156	
Boiling point, °C	> 140	(MITI 1992)
Log octanol/water coefficient, log Pow	1.82	(van Leeuwen et al. 1985)
Other physicochemical properties	Insoluble in water.	

ST

Half-life in water, days	9.5 at pH 3.8 (van Leeuwen et al. 1985) 108 at pH 5.7 (van Leeuwen et al. 1985) 1123 at pH 7.0 (van Leeuwen et al. 1985) 3316 at pH 8.0 (van Leeuwen et al. 1985) Fresh water: 47 pH7, after 200d 5.2% remaining, 0.39 = 9.4 hours, pH3.5 (WHO 1988)
Total degradation in soil	Soil, 100 mg/kg, persistence 4 weeks; soil 1000 mg/kg, persistence > 32 weeks (Chinn 1973).
Total degradation in water	Sea water, after 8 months, 20% remaining (Odeyemi 1980). Biodegradation: 2.8% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Degradation and transformation products	Dimethyldithiocarbamate – forms complexes with heavy metals, e.g. ziram. – Carbondisulfide, strong odour; threshold 0.0026 mg/l. – Dimethylamine, in presence of nitrite carcinogenic nitrosoamines are formed (Rajagopal et al. 1984).
Other information about degradation	Chemical change to dimethyldithiocarbamate which is degraded to dimethylamine and carbondisulfide by micro-organisms (Rajagopal et al. 1984). Municipal waste water, degradation in 12 days (Odeyemi 1980).
Metabolism in mammals	Absorbed lightly via skin, mucous membrane, lungs and in alimentary canal and is metabolized via different mechanisms: e.g. glucuronide conjugates, carbondisulfide, formaldehyde and dimethylamine (Anon. 1989).
Bioconcentration factor, fishes	1.1–4.4 6w, Cyprinus carpio, conc 0.025 mg/l < 3.4 6w, Cyprinus carpio, conc 0.0025 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987) (tetramethylthiuram disulfide). Low bioaccumulative (van Leeuwen et al. 1986).
LD50 values to mammals in oral exposure, mg/kg	560 orl-rat (Lewis & Sweet 1984) 210 orl-rbt (Lehman 1951) 780–865 orl-rat (Worthing & Walker 1983) 230 orl-cat (WHO 1988)
Effects on the reproduction of mammals	Rat, effects on reproduction, NOEC, 48 mg/kg in diet (Lowy et al. 1979).
Other information about mammals	Mink, NOEC, 24 weeks, < 45 mg/kg in diet – polecat, NOEC, 20 weeks, 8 mg/kg in diet (Hornshaw et al. 1987).
Health effects	Toxic by ingestion and inhalation, irritant to skin and eyes (Sax & Lewis 1987).
Carcinogenicity	Carcinogenic effects only in combination with nitrate (N-nitroso-compounds) (WHO 1988).
Mutagenicity	Generally no mutagenic effect (WHO 1988).
LD50 values to birds in oral exposure, mg/kg	300 orl-Agelaius phoeniceus > 100 orl-Passer domesticus > 100 orl-Quiscalus quiscula (Schafer et al. 1983)
Effects on the physiology of bird	Chicken, 178 mg/kg, 20 weeks, decreased growth; injuries of genitals, nervous system, e.g. paralysis (Rasul & Howell 1974).

EC50 values to microorganism, mg/l	0.1 18	15 min Microtox (van Leeuwen et al. 1985) Nitrification (van Leeuwen et al. 1985)
EC50 values to algae, mg/l	1	96hr, rpd, Chlorella pyrenoidosa (van Leeuwen et al. 1985)
LC50 values to crustaceans, mg/l	0.21	48hr, Daphnia magna (van Leeuwen et al. 1985)
	1.3	act, Daphnia pulex (Frear & Boyd 1967)
	0.008	21d, srv, grw, Daphnia magna (van Leeuwen et al. 1985b)
EC50 values to crustaceans, mg/l	0.00006	Daphnia magna (Knie et al. 1983)
LOEC values to crustaceans, mg/l	0.01 0.0018	21d, rpd, Daphnia magna 21d, grw, Daphnia magna (van Leeuwen 1986)
LC50 values to fishes, mg/l	0.23 4 0.13	48hr, Lepomis macrochirus, 48hr, Cyprinus carpio, 48hr, Salmo gairdneri, (Pesticide Manual 1983)
	0.27	96hr, Poecilia reticulata (van Leeuwen et al. 1985)
	0.007	96hr, Rasbora (Tooby et al. 1975)
	0.26	24hr, Salmo gairdneri (WHO 1988)
	0.0011	60d, Salmo gairdneri (van Leeuwen 1986)
	0.19	48hr, Oryzias latipes (MITI 1992)
EC50 values to fishes, mg/l	0.00064	Salmo gairdneri, teratogenic effects (van Leeuwen 1986)
NOEC values to fishes, mg/l	0.00032	Salmo gairdneri, embryo, grw (van Leeuwen 1986)
Effects on the physiology of water organisms	Salmo gairneri, disturbances in the ionbalance of blood and the enzyme activity of liver – cytotoxic (van Leeuwen et al. 1986).	
Other information about water organisms	LC50 (96hr) 0.39–1.01 mg/l, Cloeon dipterum (Seuge & Bluzat 1983). LC50 (96hr) 3–35 mg/l, Lymnea stagnalis (Bluzat et al. 1983). LOEC 0.3 mg/l, Colpidium campylum (Dive et al. 1980). Bakteria: Photobacterium, EC50, 15 min, 0.10 mg/l (van Leeuwen 1986).	
Other information	Dithiocarbamates induce reorganising of metals in certain organs, e.g. heart and seems to have an effect on enzymes containing metals (WHO 1988).	

1886 • Thymol

89-83-8

Synonyms	Isopropyl-m-cresol Thymic acid	
Sumformula of the chemical	C10H14O	
Use	Perfumery, mold and mildew preventive, microscopy, preservative, antioxidant, flavoring, lab reagent, synthetic menthol.	
State and appearance	White crystals.	
Odour	Aromatic odour and taste.	
Specific gravity (water=1)	0.979	
Melting point, °C	48 51	48–51 °C
Boiling point, °C	233	
Log octanol/water coefficient, log Pow	3.3	(Anon. 1986)

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Other physicochemical properties	Soluble in alcohol, carbon disulfide, chloroform, glacial acetic acid, ether and fixed or volatile oils; slightly soluble in water and glycerol. Combustible.

1887 • Tin compounds 7440-31-5

Molecular weight	118.69	
LC50 values to crustaceans, mg/l	42	21d, Daphnia magna
	55	48hr, with food, D.magna (Biesinger & Christensen 1972)
	10	144hr, Gammarus lacustris
	10	192hr, Gammarus pulex (Zencirci 1980)
EC50 values to crustaceans, mg/l	1.5	21d, rpd, Daphnia magna (Biesinger & Christensen 1972)
LOEC values to crustaceans, mg/l	0.35	21d, rpd, Daphnia magna (Biesinger & Christensen 1972)
LC50 values to fishes, mg/l	0.42	28d, Salmo gairdneri (Birge et al. 1980)

1888 • Titanium and titanium compounds 7440-32-6

LC50 values to fish, mg/l	7.31	28d, Salmo gairdneri (Birge et al. 1980)

1889 • Titanium oxide 13463-67-7

Synonyms	Tioxide Titanium dioxide	
Sumformula of the chemical	O2Ti	
Molecular weight	79.9	
TCLo values to mammals in inhalation exposure, mg/kg	250	ihl-rat, tumorigenic (Sweet 1987)
Other information about mammals	Skin and eye irritation data: skin, human 0.3 mg, mild (Sweet 1987).	
Carcinogenicity	NCI carcinogenesis bioassay (feed); no evidence: mouse, rat (Sweet 1987).	
LD50 values to birds in oral exposure, mg/kg	100	orl-Agelaius phoeniceus (Schafer et al. 1983)

1890 • Toluene 108-88-3

Synonyms	Methylbenzene Phenylmethane Methacide Toluol
Sumformula of the chemical	C7H8
Purity, %	100

ST

Use	Manufacturing of benzene derivates, caprolactam dyes, TNT; solvent recovery plants, component of gasoline; active ingredient in fungicides. Dyes, explosives, organic compounds, solvent manufacturing, benzaldehyde and benzoic acid extractant. Intermediate (75%).
State and appearance	Colourless liquid.
Odour	Aromatic odour. Odour detectable at 0.17–1.74 ppm in air (Sax 1986). Lower odour threshold; 0.25 ppm (Sax 1986). Quality: sour, burnt Hedonic tone: unpleasant to neutral Threshold odour concentration absolute: 0.17 ppm 50% recognition: 1.74 ppm 100% recognition: 1.74 ppm Odour index 100% recognition: 16 609 (Hellman & Small 1974).
Molecular weight	92.15
Specific gravity (water=1)	0.866
Vapour density (air=1)	3.14
Vapour pressure, mmHg	22 20 °C
Water solubility, mg/l	515 20 °C 470 25 °C 534.3 25 °C (Schwarz 1977) 100 (MITI 1992)
Melting point, °C	-95 (Suntio et al. 1988) -94.991 (MITI 1992)
Boiling point, °C	110.626 (MITI 1992)
Flashing point, °C	6
Log octanol/water coefficient, log Pow	2.69 (Anon. 1986) (Chin et al. 1986) 2.11-2.73 (Sabljic 1987) 2.65 (Anon. 1988) 2.69 (Schwarzenbach & Westall 1981) 2.69 (Schwarzenbach et al. 1983) 2.69 (Fuita et al. 1964) 2.73 (Hansch & Leo 1979) 2.8 (Hansch & Leo 1979) 2.21 (Banerjee et al. 1980) 2.73 (Sangster 1989)
Log soil sorption coefficient, log Kom	2.39 observed (Sabljic 1987) 2.32 calculated (Sabljic 1987)
Henry's law constant, Pa x m³/mol	460 (Anon. 1988) 673 exptl. (Mackay et al. 1979) 644 calc. (Yaws et al. 1991)
Volatilization	Relative volatility (nBuAc=1) = 2.0
Mobility	Equilibrium distribution: *mass %* air 99.34 water 0.62 solid 0.04 (Anon. 1988).

ST

Chemical oxygen demand, g 02/g	2.52 5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	2.15 5 days (Bridie et al. 1979)
Total degradation in water	Biodegradation: 112–129% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992)
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
Other information about degradation	Biodegrades with acclimated seed. Half-life is less than saturated solution (top meter) is 30.6 M as a result of evaporation. 70% evaporates with first 0.01% of water. Sewage seed has no effect (Sax 1986). Degradation of toluene: (see table below)

Degradation of toluene:

ENVIRONMENT	*INIT.CONC mg/l*	*REDOX-COND.*	*TEMP. °C*	*DEGRADATION %/day*	*REF.*
water	5	aerobic	25	100/7	a
water	10	aerobic	25	100/7	a
water	0.205	aerobic	–	95/17	b
groundwater	0.002	aerobic	13	100/8	c
groundwater	10	aerobic	10	100/10	d
groundwater	0.40	aerobic	10–13	90/1	e
groundwater	0.69	aerobic	10–13	91/2	e
groundwater	0.61	aerobic	10–13	100/3	e
groundwater	0.58	aerobic	10–13	100/5	e
sludge	appr. 50	anaerobic	35	0/56	f
sludge	appr. 50	anaerobic	35	0/56	f
soil	0.547	methanogen	17	87/42	g
soil	0.547	methanogen	17	> 99/840	g
sterile soil	0.547	methanogen	17	0/280	g
sterile soil	0.547	methanogen	17	33/840	g

a) Tabak et al. 1981
b) Batterman 1984
c) Jamison et al. 1976
d) Kappeler & Whurman 1978
e) Jensen et al. 1985
f) Horowitz et al. 1982
g) Wilson et al. 1986
(Anon. 1987b).

LD50 values to mammals in oral exposure, mg/kg	5000 orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	12124 skn-rbt (Lewis & Sweet 1984) 1.12 ipr-mus (Sax 1986)
LC50 values to mammals in inhalation exposure, ppm	5320 8hr, ihl-mus (Sax 1986)
LDLo values to mammals in non-oral exposure, mg/kg	800 ipr-rat (Sax 1986)
LCLo values to mammals in inhalation exposure, ppm	1600 ihl-gpg (Lewis & Sweet 1984) 4hr, ihl-rat (Sax 1986) ihl-gpg (Lewis & Sweet 1984) 4hr, ihl-rat (Sax 1986) 4000 ihl-gpg (Lewis & Sweet 1984) 4hr, ihl-rat (Sax 1986)

TDLo values to mammals in oral exposure, mg/kg	Teratogenic data: 9000 orl-mus, 6-15d preg. 15000 orl-mus, 6-15d preg. 30000 orl-mus, 6-15d preg. (Sax 1986)
TCLo values to mammals in inhalation exposure, mg/kg	Teratogenic data: 1500 ihl-rat, 24hr, 1-8d preg. 1000 ihl-rat, 24hr, 7-14d preg. 500 ihl-mus, 24hr, 6-13d preg. (Sax 1986)
TCLo values to mammals in inhalation exposure, ppm	200 ihl-hmn 100 ihl-man (Lewis & Sweet 1984) 1000 ihl-mus, 6hr, teratogenic effect 2–17d preg. (Sax 1986)
Health effects	200–500 ppm may cause headache, nausea and giddiness. – Irritation to rabbit belly grade 4, some capillary injection diluted; no warning properties. Eye irritation grade 6, severe burn from > 0.005 ml. – Narcotic in high concentrations. 8hr exposure to 200 ppm may cause impairment of coordination and reaction time (Sax 1986). Moderately toxic when ingested or inhaled. Slightly hazardous when absorbed through skin (Sax 1986). Skin and eye irritation data: eye, hmn, 300 ppm; skn, rbt, 435 mg, mild; skn, rbt, 500 mg, moderate; eye, rbt, 0.870 mg, mild; eye, rbt, 2 mg, 24hr, severe; eye, rbt, 100 mg/30S rns, mild (Sax 1986).
Mutagenicity	Mutagen data: dns, esc, 1 pph; dns, omi, 1 pph, 15M-C; cyt, smc, 2.4 mmol/tube; oms, grn, ihl, 562 mg/l; dnd, rat, lvr, 0.030 mmol/l; cyt, rat, ihl, 5.4 mg/m³, 16E-I; cyt, rat, scu, 12 g/kg, 12D-I; mnt, mus, orl 137600 mg/kg (Sax 1986).
Effects on amphibia	LDLo, scu, frog, 920 mg/kg (Sax 1986).
Effects on plants	Toluene had a significant germination effect on corn and soybeans seeds at 2000 ppm (dry soil basis) (Overcash et al. 1982).
Maximum longterm immission concentration in air for plants, mg/m³	20 VDI 2306
Maximum longterm immission concentration in air for plants, ppm	5 VDI 2306
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 29 mg/l (Bringmann & Kühn 1980a)
Effects on wastewater treatment	> 0.05% inhibited sewage sludge digestion (Sax 1986).

ST

EC50 values to microorganism, mg/l	18	15 min Microtox (Hermens et al. 1985)
LOEC values to algae, mg/l	105	rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
EC50 values to crustaceans, mg/l	19.6	mbt, 48hr, Daphnia magna (Pearson et al. 1979)
LC50 values to fishes, mg/l	0.02	96hr, Salmo gairdneri (Black et al. 1982)
	0.0054	96hr, sfd, Morone saxatilis juv.
	0.0076	1%., Morone saxatilis juv. (Palawski et al. 1985)
	58	24hr, Carassius auratus (Bridie et al. 1979)
	24	96hr, Lepomis macrochirus (Pickering & Henderson 1966)
	7.3	96hr, Morone saxatilis (Verschueren 1983)
	6.41	96hr, Oncorhynchus gorbusha (Korn et al. 1979)
	13	96hr, Lepomis macrochirus (Buccafusco et al. 1981)
	12.6	96hr, Pimephales promelas (Pearson et al. 1979)
LOEC values to fishes, mg/l	6.7	eggs, schr, Cyprinodon variegatus (Ward & Parrish 1980)
Effects on the physiology of water organisms	Tilapia mossambica, 45 mg/l, 4 d, change in enzyme activity (Dange 1986).	
Other information about water organisms	61 mg/l, 1hr, sunfish, lethal; 120 mg/l, Scenedesmus, inhibitor; 10 mg/l, Macrocystis pyrifera, inhibitory; 60 mg/l, Daphnia, threshold; 22–65 mg/l, 1hr, sunfish, lethal; 10 mg/l, Giant kelp, red photosynthesis; 1 mg/l, mussel, no lethal effect (Sax 1986). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): > 400 mg/l protozoa (Entosiphon sulcatum): 456 mg/l (Bringmann & Kühn 1980a)	
Other information	Emits toxic vapours when heated. May contain toxic benzene impurities. May produce BOD. Moderately toxic to fish (Sax 1986). Air pollution high (Sax 1986). Toluene can be oxidized in air to form phenol, but the reaction generally requires catalysis (Sax 1986).	

1891 • 4-Toluene sulfonic acid 104-15-4

ST

Synonyms	p-Toluenesulfonic acid p-Toluenesulfonate
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

1892 • 2,4-Toluenediisocyanate 584-84-9

Synonyms	Cresorcinol diisocyanate 2,4-Diisocyanato-1-methylbenzene 2,4-Diisocyanatotoluene Isocyanic acid, methylphenylene ester Isocyanic acid, 4-methyl-m-phenylene ester Toluene diisocyanate Toluene-2,4-diisocyanate 2,4-TDI	
Sumformula of the chemical	$C_9H_6N_2O_2$	
State and appearance	White liquid.	
Odour	Characteristic, medicated bandage, pungent. Odour index: 6 (Verschueren 1983).	
Molecular weight	174.16	
Specific gravity (water=1)	1.2	
Vapour density (air=1)	6	
Conversion factor, 1 ppm in air=	7.24	mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.14	ppm
Vapour pressure, mmHg	0.01 1	20 °C 80 °C
Melting point, °C	21	
Boiling point, °C	251	
LD50 values to mammals in oral exposure, mg/kg	5800	orl-rat (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	56	ipr-mus (Sweet 1987)
LC50 values to mammals in inhalation exposure, ppm	13 10 14 11	ihl-gpg, 4hr ihl-mus, 4hr ihl-rat, 4hr (Sweet 1987) ihl-rbt, 4hr/day, 14 days (Verschueren 1983)
TCLo values to mammals in inhalation exposure, ppm	0.02 0.5	ihl-hmn, 2 years, lungs, thorax or respiration ihl-hmn, sense organs and special senses lungs, thorax or respiration (Sweet 1987)
Other information about mammals	Skin and eye irritation data: skin, rabbit, 500 mg open, severe; skin, rabbit, 500 mg, 24hr, moderate; eye, rabbit, 100 mg, severe (Sweet 1987).	
Health effects	Eye and nose irritation; 0.1 ppm, 30 min; no effect level: 0.01 ppm, 30 min (Verschueren 1983).	
Mutagenicity	Mutation data: microsomal assay; Salmonella typhimurium, 0.5 mg/plate (Sweet 1987).	

ST

LD50 values to birds in oral exposure, mg/kg	100 100 > 100	orl-bdw (Sweet 1987) orl-Agelaius phoeniceus orl-Sturnus vulgaris (Schafer et al. 1983)
Maximum longterm immission concentration in air for plants, mg/m^3	0.007	VDI 2306
Maximum longterm immission concentration in air for plants, ppm	0.001	VDI 2306

1893 • 2,6-Toluenediisocyanate 91-08-7

Synonyms	2,6-Diisocyanatotoluene 2,6-TDI 2,6-Diisocyanato-1-methylbenzene Isocyanic acid, 2-methyl-meta-phenylene ester 2-Methyl-meta-phenyleneisocyanate Toluene-2,6-diisocyanate Toluene diisocyanate	
Sumformula of the chemical	C9H6N2O2	
Odour	USSR: human odour perception: human reflex response: animal chronic exposure: (Verschueren 1983).	non perception: 0.15 mg/m^3; perception: 0.020 mg/m^3; no response: 0.050 mg/m^3; adverse response: 0.1 mg/m^3; no effect: 0.02 mg/m^3; adverse effect: 0.2 mg/m^3
Molecular weight	174.17	
Conversion factor, 1 ppm in air=	7.24	mg/m^3
Conversion factor, 1 mg/m^3 in air=	0.14	ppm
LC50 values to mammals in inhalation exposure, mg/m^3	91	4hr, ihl-mus (Lewis & Sweet 1984)
TCLo values to mammals in inhalation exposure, ppm	0.08 0.05	ihl-hmn (Lewis & Sweet 1984) ihl-hmn, sense organs and special senses lungs, thorax or respiration (Sweet 1987)
Mutagenicity	Mutation data: microsomal assay; Salmonella typhimurium, 0.010 mg/plate (Sweet 1987).	
LD50 values to birds in oral exposure, mg/kg	100 100 ≥ 100	orl-bdw (Sweet 1987) orl-Agelaius phoeniceus orl-Sturnus vulgaris (Schafer et al. 1983)
Maximum longterm immission concentration in air for plants, mg/m^3	0.007	VDI 2306
Maximum longterm immission concentration in air for plants, ppm	0.001	VDI 2306

ST

LC50 values to fishes, mg/l	164 96hr, Pimephales promelas (Curtis et al. 1979)
Other information about water organisms	Grass shrimp (Palaemonetes pugio): no significant mortality below 508 mg/l (Verschueren 1987).

1894 • 4-Toluenesulfonamide

70-55-3

Synonyms	p-Toluenesulfonamide
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to birds in oral exposure, mg/kg	75 orl-Agelaius phoeniceus 75 orl-Sturnus vulgaris (Schafer et al. 1983)

1895 • o-Toluenesulfonamide

88-19-7

Sumformula of the chemical	C7H9NO2S
EINECS-number	2018088
Water solubility, mg/l	1600 25° (MITI 1992)
Melting point, °C	155–156 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradation	Confirmed to be non–biodegradable (Anon. 1987).
Bioconcentration factor, fishes	0.4–0.9 6w, Cyprinus carpio, conc 3 mg/l < 1–2.6 6w, Cyprinus carpio, conc 0.3 mg/l (MITI 1992)
LC50 values to fishes, mg/l	335 48hr, Oryzias latipes (MITI 1992)
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).

1896 • m-Tolyl N-methylcarbamate

1129-41-5

Sumformula of the chemical	C9H11O2N
Water solubility, mg/l	> 1000 (MITI 1992)
Melting point, °C	74–75 (MITI 1992)
Total degradation in water	Biodegradation: 36–41% (NO2) by BOD (on the upward trend) Period: 28d Substance: 100 mg/l Sludge: 30 mg/l (MITI 1992).

1897 • Toxaphene *

8001-35-2

Synonyms	Camphechlor
Sumformula of the chemical	C10H10Cl8 * on an average

ST

Chemicals in the product	* Toxaphene is composed of; chlorinated bicyclic terpenes; * mainly; chlorinated camphene; * (Lewis & Sweet 1984)
Use	Pesticide, insecticide (on cotton crops).
State and appearance	Amber, waxy solid.
Odour	Mild odour of chlorine and camphor.
Molecular weight	413.8
Water solubility, mg/l	0.5–3 25 °C
Melting point, °C	65–90
Log octanol/water coefficient, log Pow	3.3 (Anon. 1989) 5.5 (Anon. 1989)
Henry's law constant, Pa x m³/mol	0.42 20 °C
Half-life in soil, days	900 (Li et al. 1990) 730 20 years (Ware 1988)
Aerobic degradation in water	Persistent in surface water (Ware 1988). Persistent in an oligotrophic lake for 6 years (Terriere et al. 1966).
Other information about degradation	Degrades in UV-light and in high temperatures (WHO 1984).
Metabolism in mammals	Absorbed through skin, lungs and alimentary canal. Is metabolized quickly, half-life in rat < 1 week, through dechlorination and oxidation and is excreted with urine, feces and milk (Ware 1988).
Bioconcentration factor, fishes	3100–91000 (Verschueren 1983) 70000–107000 150d, Pimephales promelas (Verschueren 1983) 91000 Ictalurus, juv (NCI 1979)
Bioconcentration factor, mollusca	2920–15200 96hr (Verschueren 1983) 9000–15200 oyster (Schimmel et al. 1977)
Bioconcentration factor, crustaceans	400–1200 96hr (Verschueren 1983) 800–1200 shrimp (Schimmel et al. 1977)
LD50 values to mammals in oral exposure, mg/kg	40 orl-rat 15 orl-dog (Lewis & Sweet 1984) 60 orl-man (IUPAC 1979)
LD50 values to mammals in non-oral exposure, mg/kg	600 skn-rat (Lewis & Sweet 1984) 60–90 ukn-rat 270 ukn-gpg 75–100 ukn-rbt 20–30 ukn-dog (Virtanen & Nuuja 1987)
LDLo values to mammals in oral exposure, mg/kg	40 orl-hmn (Lewis & Sweet 1984)
Effects on the physiology of mammals	Dog, injuries in kidneys, LOEL, 4 mg/kg/d; rat, injuries in liver, LOEL, 1.25 mg/kg/d (Ware 1988).
Health effects	Convulsions in human at 10 mg/kg (Virtanen & Nuuja 1987). Toxic by ingestion, inhalation, skin absorption; most uses prohibited (Sax & Lewis 1987). USA, acceptable daily intake for human (ADI): 0.00125 mg/kg (NAS 1977).

Carcinogenicity	NCI carcinogenesis bioassay completed: results positive: mus; results indefinite, rat (Lewis & Sweet 1984).	
Mutagenicity	Positive in Ames test (Ware 1988).	
LD50 values to birds in oral exposure, mg/kg	31	orl-dck (Lewis & Sweet 1984)
Effects on bees	LD50, 48hr, 0.000144 mg/bi (Torchio 1973).	
EC50 values to algae, mg/l	0.01	10d, Phaeodactylum (Verschueren 1983)
	0.38	Selenastrum (USEPA 1980)
LOEC values to algae, mg/l	0.01	rpd, schr, Phaedactylum tricornutum (Walsh 1972)
LC50 values to crustaceans, mg/l	0.015	48hr, Daphnia magna (Sanders & Cope 1966, Frear & Boyd 1967)
	0.0000072	96hr, Acartia tonsa (Khattat & Farley 1976)
	0.006	96hr, Gammarus fasciatus (Sanders 1972)
	0.01	48hr, Simocephalus serrulatus (Verschueren 1983)
	0.0014	96hr, Penaeus duorarum (Schimmel et al. 1977)
	0.015	act, Daphnia pulex (Kenaga 1979)
EC50 values to crustaceans, mg/l	0.016	96hr, Crassostrea (Shimmel et al. 1977)
NOEC values to crustaceans, mg/l	0.00007	21d, Daphnia magna (Sanders 1980)
LC50 values to fishes, mg/l	0.008 0.004	96hr, Salmo gairdneri 96hr, Lepomis macrochirus (Edwards 1977)
	0.0011 0.0005	96hr, Cyprinodon 96hr, Lagodon rhomboides (Schimmel et al. 1977)
	0.0055 0.003 0.012	96hr, Salmo gairdneri 96hr, Salmo trutta m. lacustris 96hr, Perca fluviatilis (Macek & McAllister 1970)
	0.018 0.011 0.014	act, Lepomis macrochirus act, Salmo gairdneri act, Pimephales promelas (Kenaga 1979)
	0.0024	96hr, Lepomis (LeBlanc 1984)
	0.0005	144hr, Leiostomus (Lowe 1964)
LOEC values to fishes, mg/l	0.0003 0.000054	grw, srv, schr, Ictalurus punctatus grw, schr, Pimephales promelas (Mayer et al. 1977)
NOEC values to fishes, mg/l	0.00013 0.000025	grw, srv, schr, Ictalurus punctatus grw, schr, Pimephales promelas (Mayer et al. 1977)
Other information about water organisms	MATC: 259d, Pimephales, 0.000025–0.000054; 240d, Ictalurus, 0.00013 –0.0003 mg/l (Mayer et al. 1977).	

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1898 • TPN-12

14759-08-6

LC50 values to fishes, mg/l	0.11 0.17	48hr, Cyprinus carpio 48hr, Carassius auratus (Hashimoto & Nishiuchi 1981)

1899 • Tremorine

51-73-0

Other information about mammals	LDfr = 70.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).	
LD50 values to birds in oral exposure, mg/kg	100 > 100	orl-Agelaius phoeniceus orl-Sturnus vulgaris (Schafer et al. 1983)

1900 • Tri-butoxyethyl phosphate

78-51-3

Sumformula of the chemical	C18H39O7P	
EINECS-number	2011229	
Water solubility, mg/l	560	(MITI 1992)
Melting point, °C	< -10	(MITI 1992)
Boiling point, °C	> 300	(MITI 1992)
Log octanol/water coefficient, log Pow	3.75	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.6–4.1 < 5.8	6w, Cyprinus carpio, conc 0.2 mg/l 6w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
LC50 values to fishes, mg/l	27.7	48hr, Oryzias latipes (MITI 1992)

1901 • S, S, S-Tributylphosphorotrithioate

78-48-8

Synonyms	Butifos Butiphos Phosphorotrithioic acid, S, S, S-tributyl ester DEF	
Sumformula of the chemical	C12H27OPS3	
Molecular weight	314.54	
LD50 values to mammals in oral exposure, mg/kg	150 260	orl-rat orl-gpg (Lewis & Sweet 1984)

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LD50 values to mammals in non-oral exposure, mg/kg	97 168 210 170 290 150	skn-rbt skn-rat ipr-rat unk-rat ipr-mus ipr-gpg (Lewis & Sweet 1984)
LD50 values to birds in oral exposure, mg/kg	> 101	orl-Agelaius phoeniceus (Schafer et al. 1983)
LC50 values to crustaceans, mg/l	0.1	96hr, Gammarus lacustris (Sanders 1969)
LC50 values to fishes, mg/l	18.78 5.6 0.31	4d, Ictalurus punctatus 4d, Ictalurus punctatus (Mather-Mihaich & Di Giulio 1986) 96hr, Salmo gairdneri (Palawski et al. 1983)
LOEC values to fishes, mg/l	0.0012 0.0036 0.0048 0.00196	grw, schr, Salmo gairdneri srv, schr, Salmo gairdneri grw, schr, Ictalurus punctatus srv, schr, Ictalurus punctatus (Cleveland & Hamilton 1983)
Effects on the physiology of water organisms	Ictalurus punctatus, 1.4 mg/l, 21 d, change in enzyme activity (Mather-Mihaich & Di Giulio 1986). Ictalurus punctatus, 0.056 mg/l, 21 d, hematological effect (change in various blood parameters such as red blood cell count, hematocrit, and serum osmolarity) (Mather-Mihaich & Di Giulio 1986).	
Other information about water organisms	LC50 (96hr) 2.1 mg/l, Pteronarcys californica (Sanders & Cope 1968).	

1902 • Tri-n-hexylchlorosilane 3634-67-1

Sumformula of the chemical	C18H39SiCl
Boiling point, °C	121–123 (MITI 1992)
Total degradation in water	Biodegradation: 0–1% by BOD (dechlorinated to Trihexylsilanol) period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

1903 • Tri-o-cresylphosphate 78-30-8

Synonyms	Tri-o-tolyl phosphate o–Tricresyl phosphate
Sumformula of the chemical	C21H2104P
Total degradation in water	Biodegradation: 65.7% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).

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LC50 values to fishes, mg/l	7000 8700	96hr, Lepomis macrochirus 96hr, Menidia audens (Dawson et al. 1977)

1904 • 1,3,5-Tri-tert-butylbenzene 1460-02-2

Sumformula of the chemical	C18H30
Water solubility, mg/l	< 100 (MITI 1992)
Melting point, °C	71–73 (MITI 1992)
Log octanol/water coefficient, log Pow	> 5.90 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	7960–25700 10w, Cyprinus carpio, conc 0.02 mg/l 9750–36700 10w, Cyprinus carpio, conc 0.002 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 200 48hr, Oryzias latipes (MITI 1992)

1905 • 2,4,6-Tri-tert-butylphenol 732-26-3

Sumformula of the chemical	C18H30O
Water solubility, mg/l	35 (MITI 1992)
Melting point, °C	128–132 (MITI 1992)
Log octanol/water coefficient, log Pow	6.06 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	4830–16000 8w, Cyprinus carpio, conc 0.01 mg/l 4320–23200 8w, Cyprinus carpio, conc 0.001 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be accumulated on a high level (Anon. 1987).
LC50 values to fishes, mg/l	128 48hr, Oryzias latipes (MITI 1992)

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1906 • Triadimefon 42121-43-3

Use	Active ingredient in fungicides.
LC50 values to fishes, mg/l	10–50 96hr, Carassius auratus (Pesticide Manual 1983)

1907 • Triallylamine 102-70-5

Sumformula of the chemical	C9H15N
EINECS-number	2030482
Water solubility, mg/l	> 500 (MITI 1992)
Melting point, °C	155–156 (MITI 1992)
Log octanol/water coefficient, log Pow	2.42 (MITI 1992)
Total degradation in water	Biodegradation: 1% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	2.0–2.8 6w, Cyprinus carpio, conc 0.1 mg/l 2.3–4.8 6w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non–accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	11.5 48hr, Oryzias latipes (MITI 1992)

1908 • Triallylphosphate 1623-19-4

Sumformula of the chemical	C9H15O4P
Water solubility, mg/l	> 1000 (MITI 1992)
Log octanol/water coefficient, log Pow	1.76 (MITI 1992)
Total degradation in water	Biodegradation: 0–41% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.1–0.9 6w, Cyprinus carpio, conc 0.1 mg/l < 1.2 6w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	48 48hr, Oryzias latipes (MITI 1992)

1909 • 2,4,6-Triamino-1,3,5-triazine 108-78-1

Synonyms	Melamine
Sumformula of the chemical	C3H6N6
EINECS-number	2036154
Water solubility, mg/l	4000 (MITI 1992)

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Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.38 < 3.8	6w, Cyprinus carpio, conc 2 mg/l 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	1000	48hr (MITI 1992)

1910 • Tribenzylphosphite 15205-57-9

Sumformula of the chemical	C21H2103P
Total degradation in water	Biodegradation: 78–80% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

1911 • Tribromoethene 598-16-13

EC50 values to algae, mg/l	3.5	48hr, grw, Chlorella pyrenoidosa (Canton & Wegman 1983)

1912 • 2,4,6-Tribromophenol 118-79-6

Water solubility, mg/l	0.07	(MITI 1992)
Melting point, °C	94–96	(MITI 1992)
Boiling point, °C	244	(MITI 1992)
Total degradation in water	Biodegradation: 49% by BOD (on the upward trend) period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LC50 values to fishes, mg/l	10 6.5–6.8 4.5–4.9	48hr, Pimephales promelas 96hr, Pimephales promelas 192hr, Pimephales promelas (Phipps et al. 1981)

1913 • 2,4,6-Tribromophenyl(2-methyl-2,3-dibromopropyl)ether 36065-30-2

Sumformula of the chemical	C10H9Br50

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Melting point, °C	81	(MITI 1992)
Boiling point, °C	280	(MITI 1992)
Total degradation in water	Biodegradation: 2.9% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	4600–20600 6800–31000	8w, Cyprinus carpio, conc 0.04 mg/l 8w, Cyprinus carpio, conc 0.004 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be accumulated on a high level (Anon. 1987).	
LC50 values to fishes, mg/l	118	48hr, Oryzias latipes (MITI 1992)

1914 • Tributyl-1,2,4-benzene tricarboxylate 1726-23-4

Sumformula of the chemical	C21H30O6	
Water solubility, mg/l	< 10	(MITI 1992)
Total degradation in water	Biodegradation: 85–92% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	

1915 • Tributylphosphate 126-73-8

Synonyms	Tri-n-butylphosphate Tributyl phosphate	
Use	Solvent; plasticiser.	
Molecular weight	266.36	
Water solubility, mg/l	400 70	20 °C (MITI 1992)
Melting point, °C	< -80	(MITI 1992)
Boiling point, °C	289	(MITI 1992)
Log octanol/water coefficient, log Pow	4	(Anon. 1988)
Henry's law constant, Pa x m³/mol	0.22	(Anon. 1988)
Mobility	Equilibrium distribution: air water solid	 *mass %* 2.90 38.32 58.79 (Anon. 1988).

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Total degradation in water	Biodegradation: 0–41% by BOD period: 14d substnce: 30 mg/l sludge: 100 mg/l (MITI 1992).
Bioconcentration factor, fishes	5.5–10 6w, Cyprinus carpio, conc 0.06 mg/l 6.9–20 6w, Cyprinus carpio, conc 0.006 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	3000 orl-rat (Lewis & Sweet 1984)
LOEC values to algae, mg/l	3.2 rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
LC50 values to fishes, mg/l	5.0–9.0 96hr, Salmo gairdneri (Dave & Lindman 1978) 42–105 120hr, Salmo gairdneri (Dave et al. 1979) 9.6 96hr, Oryzias latipes 8.8 96hr, Carassius auratus (Sasaki et al. 1981) 14.2 48hr, Oryzias latipes (MITI 1992)
Other information about water organisms	EC50 (24hr) 20 mg/l, rpd, Tetrahymena pyriformis (Yoshioka et al. 1985).

1916 • Tributyltin acetate 56-36-0

Other information about mammals	LDfr = 37.5 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).
EC50 values to algae, mg/l	0.00036 grw, 72hr, Skeletonema costatum (Walsh et al. 1985)

1917 • Tributyltin benzoate 4342-36-3

Other information about mammals	LDfr = 37.5 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

1918 • Tributyltin chloride 1461-22-9

Synonyms	Chlorotributylstannane
LD50 values to birds in oral exposure, mg/kg	75.0–100 orl-Agelaius phoeniceus 100 orl-Passer domesticus (Schafer et al. 1983)
EC50 values to algae, mg/l	0.00036 72hr, grw, Skeletonema costatum (Walsh et al. 1985)

1919 • Tributyltin fluoride 1983-10-4

LC50 values to crustaceans, mg/l	0.002 96hr, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	0.006–0.008 96hr, Alburnus alburnus (Linden et al. 1979)

1920 • Tributyltin hydroxide 1067-97-6

Sumformula of the chemical	C12H28OSn	
Bioconcentration factor, fishes	2500–9210 1830–7510	8w, Cyprinus carpio, conc 0.0005 mg/l 8w, Cyprinus carpio, conc 0.00005 (MITI 1992)
LC50 values to fishes, mg/l	0.0228	48hr, Oryzias latipes (MITI 1992)

1921 • Tributyltin hydroxyacetate 5847-48-3

Other information about mammals	LDfr = 12.5 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

1922 • Tributyltin laurate 3090-36-6

Sumformula of the chemical	C24H30O2Sn	
Water solubility, mg/l	1.2	(MITI 1992)
Melting point, °C	23.5	(MITI 1992)
Total degradation in water	Biodegradation: 35% by BOD (Bioaccumultion test was carried out to tributyltin hydroxide) period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

1923 • Tributyltin neodecanoate 28801-69-6

Other information about mammals	LDfr = 25.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

1924 • Tributyltin oxide 56-35-9

Synonyms	Bis(tributyltin)oxide Hexabutyldistannoxane Bis(tributyloxide) of tin Bis(tributylstannyl)oxide Hexabutylditin Oxybis(tributyltin)	
Sumformula of the chemical	C24H54OSn2	
Use	Bactericide, fungicide.	
Molecular weight	596.16	
Water solubility, mg/l	50	(MITI 1992)
Boiling point, °C	180	
Log octanol/water coefficient, log Pow	3.31	(MITI 1992)

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Total degradation in water	Biodegradation: 2% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992)	
Bioconcentration factor, fishes	2550–12100 2880–11200	12w, Cyprinus carpio, conc 0.0005 mg/l 12w, Cyprinus carpio, conc 0.00005 mg/l (MITI 1992)
Other information about bioaccumulation	Bis(tributyltin)oxide confirmed to be accumulated on a high level (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	87 55	orl-rat orl-mus (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	900 12.5 7.21 6 11700 11700 900	skn-rbt (Lewis & Sweet 1984) ipr-mus ipr-rat ivn-mus scu-rat skn-rat skn-rbt (Sweet 1987)
LDLo values to mammals in oral exposure, mg/kg	50	orl-rbt (Sweet 1987)
LD50 values to birds in oral exposure, mg/kg	30	orl-Agelaius phoeniceus (Schafer et al. 1983)
LC50 values to algae, mg/l	0.016	pht, Selenastrum quadricauda (Wong et al. 1982)
LC50 values to crustaceans, mg/l	0.002	96hr, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	0.027 0.015 0.031 0.053 0.0208	24hr, Salmo gairdneri (Kemp et al. 1979) 96hr, Alburnus alburnus (Linden et al. 1979) 24hr, Salmo gairdneri 96hr, Sarotherodon (Chliamatovitch & Kuhn 1977) 48hr, Oryzias latipes (MITI 1992)
Effects on the physiology of water organisms	Poecilia reticulata: 0.00032 mg/l, 90 d, change in length and/or weight; 0.00001 mg/l, 30 d, histological effect (presence of physical damage to tissues) (Wester & Canton 1987).	

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1925 • 1,1,1-Trichloro-2-methyl-2-propanol 57-15-8

Sumformula of the chemical	C4H7Cl3O	
EINECS-number	2003176	
Water solubility, mg/l	> 2500	(MITI 1992)
Melting point, °C	76–79	(MITI 1992)
Log octanol/water coefficient, log Pow	1.73	(MITI 1992)

Total degradation in water	Biodegradation: 9–17% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	1.5–2.4 6w, Cyprinus carpio, conc 1 mg/l < 1.7 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	127 48hr, Oryzias latipes (MITI 1992)

1926 • Trichloroacetaldehyde 75-87-6

Synonyms	Trichloroethanal
Sumformula of the chemical	C2HOCl3
Use	Manufacture of DDT; organic synthesis.
State and appearance	Colourless liquid.
Odour	Characteristic: sweet. Threshold Odour Concentrations: Population Identification Threshold (PIT50%): 0.047 ppm Population Identification Threshold (PIT100%): 0.047 ppm Odour Index: at 20 °C: 980000 recognition: 0.035–0.050 mg/m³ (hydrate) (Verschueren 1983).
Molecular weight	147.4
Specific gravity (water=1)	1.512 at 20/4 °C
Vapour density (air=1)	5.1
Conversion factor, 1 ppm in air=	6 mg/m³
Conversion factor, 1 mg/m³ in air=	0.166 ppm
Vapour pressure, mmHg	35 20 °C
Water solubility, mg/l	30000 (MITI 1992)
Melting point, °C	-58– -57 (MITI 1992)
Boiling point, °C	98 (MITI 1992)
Total degradation in water	Biodegradation: 2–12% by BOD, oxidized to Trichloroacetic acid period: 28d substance: 100 mg/l sludge: 30mg/l (MITI 1992).
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	50–400 orl-rat (Patty 1967)
LD50 values to birds in oral exposure, mg/kg	> 100 orl-Agelaius phoeniceus (Schafer et al. 1983)

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Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): hydrate: Bacteria (Pseudomonas putida): 1.6 mg/l (Bringmann & Kühn 1980).
LOEC values to algae, mg/l	2.8 rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
Other information about water organisms	LOEC 79 mg/l, rpd, schr, Entosiphon sulcatum (Bringmann & Kühn 1980a). Toxicity threshold (cell multiplication inhibition test): hydrate: algae (Microcystis aeruginosa): 78.0 mg/l (Bringmann & Kühn 1976) green algae (Scenedesmus quadricauda): 2.8 mg/l protozoa (Entosiphon sulcatum): 79 mg/l protozoa (Uronema parduczi): 86 mg/l (Bringmann & Kühn 1980).

1927 • Trichloroacetic acid 76-03-9

Synonyms	TCA Trichloroethanoic acid	
Sumformula of the chemical	C2HCl3O2	
Use	Herbicide.	
Molecular weight	163.4	
Water solubility, mg/l	> 2000	(MITI 1992)
Melting point, °C	57.5	(MITI 1992)
Boiling point, °C	197.5	(MITI 1992)
pKa	0.65	
Log octanol/water coefficient, log Pow	1.7	
Total degradation in water	Biodegradation: 0–46% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	0.4–1.0 < 1.7	6w, Cyprinus carpio, conc 0.2 mg/l 6w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	5640 5000	orl-mus orl-rat (Lewis & Sweet 1984)
LDLo values to mammals in non-oral exposure, mg/kg	500	ipr-mus (Lewis & Sweet 1984)
LOEC values to algae, mg/l	200 250	rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a) rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to crustaceans, mg/l	2000 4800	48hr, Daphnia magna (Dennis et al. 1979) 96hr, 10 °C, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	2000 9300 277	96hr, Pimephales promelas (Dennis et al. 1979) 96hr, 10 °C, Alburnus alburnus (Linden et al. 1979) 48hr, Oryzias latipes (MITI 1992)

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1928 • 2,3,4-Trichloroacetophenone 13608-87-2

LC50 values to fishes, mg/l	2	96hr, Pimephales promelas (Veith et al. 1983)

1929 • 2,3,5-Trichloroaniline 18487-39-3

LC50 values to fishes, mg/l	1.4	14d, Poecilia reticulata (Hermens et al. 1984)

1930 • 2,4,5-Trichloroaniline 636-30-6

LC50 values to fishes, mg/l	2	14d, Poecilia reticulata (Hermens et al. 1984)

1931 • 2,4,6-Trichloroaniline 634-93-5

Water solubility, mg/l	40	(MITI 1992)
Melting point, °C	78.5	(MITI 1992)
Boiling point, °C	262	(MITI 1992)
Log octanol/water coefficient, log Pow	3.9	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	27–112 52–147	8w, Cyprinus carpio, conc 0.1 mg/l 8w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	1–10 8.2	96hr, Pimephales promelas (Könemann 1979) 48hr, Oryzias latipes (MITI 1992)

1932 • Trichlorobenzene 12002-48-1

Sumformula of the chemical	C6H5Cl3	
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	440–1810 550–1540	8w, Cyprinus carpio, conc 0.056 mg/l 8w, Cyprinus carpio, conc 0.0056 mg/l
LC50 values to fishes, mg/l	5.6	48hr, Oryzias latipes (MITI 1992)

1933 • 1,2,3-Trichlorobenzene 87-61-6

Synonyms	VIC-Trichlorobenzene V-Trichlorobenzene 1,2,6-Trichlorobenzene
Sumformula of the chemical	C6H3Cl3
Use	Not used directly in any quantity. Used as intermediate in chemical synthesis. Solvent for high melting products, coolant in electrical installations and glass tempering, polyester dyeing, termite preparations, synthetic transformer oil, lubricants, heat transfer medium, and insecticides.
State and appearance	Colourless plates. Will sink in water and be found on bottom (Sax 1986). White crystals. Insoluble in water.
Molecular weight	181.44
Specific gravity (water=1)	1.69
Vapour density (air=1)	6.26
Vapour pressure, mmHg	0.07 at 25 °C 1 at 40 °C
Water solubility, mg/l	12 22 °C 12.27 25 °C (Miller et al. 1984) 18 25 °C (Banerjee 1984)
Melting point, °C	53 (Suntio et al. 1988) 53–54 (MITI 1992)
Boiling point, °C	218–219 (MITI 1992)
Log octanol/water coefficient, log Pow	4.1 (Anon. 1988) 4.05 (Schwarzenbach & Westall 1981) 4.27 (Hansch & Leo 1979) 4.11 (Konemann et al. 1979) 4.2 (Konemann et al. 1979) 4.05 (Wateral et al. 1982) 4.02 (McDuffie 1981) 4.04 Miller (et al. 1984) 4.14 (Chiou 1985) 4.11 (Hawker & Connell 1985)
Log soil sorption coefficient, log Kom	3.37 observed (Sabljic 1987) 2.77 calculated (Sabljic 1987)
Henry's law constant, Pa x m³/mol	420 (Anon. 1988) 234 calc. (Suntio et al. 1988) 127 exptl. (Suntio et al. 1988)
Mobility	Equilibrium distribution: *mass %* air 97.99 water 0.69 solid 1.32 (Anon. 1988).
Other physicochemical properties	Flammability: slight, Combustion requires preheating. Moderate hazard. Insoluble.
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Other information about degradation	Biodegradation by Pseudomonas: 200 mg/l, 30 °C: parent: 87% ring disruption in 120 hours mutant: 100% ring disruption in 43 hours (Verschueren 1983).
Bioconcentration factor, fishes	350–980 6w, Cyprinus carpio, conc 0.025 mg/l 130–1200 6w, Cyprinus carpio, conc 0.0025 mg/l (MITI 1992)
Other information about bioaccumulation	May accumulate similar to chlorinated pesticides. Biological half-life is 2 days. The major metabolite in the rabbit is 2,3,4-trichlorophenol (Sax 1986). Confirmed to be accumulated on a medium level (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	756 orl-rat 766 orl-mus (Sax 1986)
LD50 values to mammals in non-oral exposure, mg/kg	6139 scu-rat (Sax 1986)
Health effects	Irritating to eyes and mucous membranes. The amount of trichlorobenzene necessary to induce a toxic reaction via application to the skin is quite high. May cause liver damage (Sax 1986).
EC50 values to microorganism, mg/l	2.5 15 min Microtox (Hermens et al. 1985) 105 0.5hr, Resazurin reduction, methanol 100 0.5hr, Resazurin reduction, ethanol 80 0.5hr, Resazurin reduction, acetone 135 0.5hr, Resazurin reduction, DMSO (Thompson et al. 1986)
EC50 values to algae, mg/l	0.9 rpd,96hr, Selenastrum capricornutum (Calamari et al. 1983) 0.9 96hr, growth, Selenastrum capricornutum 2.2 3h, photosynthesis, Selenastrum capricornutum (Calamari et al. 1983)
LC50 values to crustaceans, mg/l	0.35 24hr, Daphnia magna (Calamari et al. 1983)
EC50 values to crustaceans, mg/l	0.93 rpd, 14d, Daphnia magna 0.35 mbt,24hr, Daphnia magna (Calamari et al. 1983)
LC50 values to fishes, mg/l	2.4 14d, Poecilia reticulata (Könemann 1979) 3.1 48hr, Branchydanio rerio 0.71 48hr, Salmo gairdneri (Calamari et al. 1983) 0.348 4d, Poecilia reticulata (Van Hoogen & Opperhuizen 1988) 12.3 48hr, Oryzias latipes (MITI 1992)
EC50 values to fishes, mg/l	0.71 srv,48hr, Salmo gairdneri (Calamari et al. 1983)
Other information about water organisms	100 mg/l, micro life, 98% kill (Sax 1986). > 10 mg/l, 48hr, hard clam eggs, LC50; > 10 mg/l, 228hr, hard clam larvae, LC50; 3.13 mg/l, 48hr, oyster eggs, LC50 (Sax 1986). LC50, 0.00192 mM/l, 4 d, Poecilia reticulata (Van Hoogen & Opperhuizen 1988).
Other information	Emits toxic vapours when heated to decomposition. – Air pollution high (Sax 1986).

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1934 • 1,2,4-Trichlorobenzene 120-82-1

Synonyms	unsym-Trichlorobenzene asym-Trichlorobenzene as-Trichlorobenzene 1,2,4-Trichlorobenzol
Sumformula of the chemical	C6H3Cl3
Use	Solvent in chemical manufacturing; dyes and intermediates; dielectric fluid; synthetic transformer oils; insecticides; herbicides; heat transfer medium; degreaser; lubricant.
State and appearance	Colourless, stable, refractive liquid; insoluble in water. Solid colourless crystals (Sax 1986).
Odour	Lower odour threshold: 0.88–2.4 ppm. – No odour at lowest level, definite odour at higher level (Sax 1986).
Molecular weight	181.44; 182
Specific gravity (water=1)	1.454
Vapour density (air=1)	1.463
Water solubility, mg/l	36 20 °C (Anon. 1989) 30 25 °C (Sax 1986) 31.3 25 °C (Banerjee 1984)
Melting point, °C	16.95 (Suntio et al. 1988) 17 (MITI 1992)
Boiling point, °C	210 (MITI 1992)
Flashing point, °C	110 93.3
Log octanol/water coefficient, log Pow	4.23 (Sax 1986) 3.98 (Chin et al. 1986) 4.18 (Anon. 1986) 3.93–4.67 (Sabljic 1987) 4.26 (Chin et al. 1986) 4.1 (Anon. 1988) 4.05 (Schwarzenbach & Westall 1981) 4.27 (Yalkowsky et al. 1979) 3.93 (Konemann et al. 1979) 3.97 (Wateral et al. 1982) 3.98 (Miller et al. 1984) 4.02 (Chiou 1985)
Henry's law constant, Pa x m³/mol	108.4 240 (Anon. 1988) 366.6 (Suntio et al 1988)
Mobility	Equilibrium distribution: *mass %* air 96.60 water 1.16 solid 2.24 (Anon. 1988).
Other reactions in atmosphere	In the troposphere reaction with OH-radicals: half-life 30 days (Rinke & Zetzsch 1984).
Hydrolysis in water	No hydrolysis in normal environmental conditions (Åkermark et al. 1976).

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Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Not easily degradable in Closed bottle test (BUA 1988).; Not easily degradable (Anon. 1989).; Confirmed to be non-biodegradable (Anon. 1987).
Other information about degradation	Photochemical dechlorination forms 1,3-dichlorobenzene and 1,4-dichlorobenzene (Åkerman et al. 1976). Degradation in anaerobic conditions has not been shown (BUA 1988). Will volatilize from water fairly rapidly: half-life of 45 minutes when aerated; 100 ppm completely volatilized from unaerated distilled water in 2 days. 50 mg/l in aerated mixed cultures of aerobic microorganisms – measurable level still detected after 9 days. Octanol/water partition coefficient suggests the possibility of adsorption to organic material. 1.7 mg/l with unacclimatized industrial wastewater microorganisms degraded 14% in 24 hours, 36% at 72 hours, and 43% in 7 days; an initial concentration of 2.6 mg/l decreased 28% in 7 days. Under environmental conditions – unacclimated microorganisms and varying carbon sources – a much lower rate of degradation is expected. Hydrolysis probably will not occur; oxidation may be possible, but unlikely to be important (Sax 1986).
Metabolism in fishes	Bluegills fed Daphnia containing 1,2,4-TCB showed only slight increase in body burden of compound, 5% of that during exposure to same level in the water (Sax 1986).
Bioconcentration factor, fishes	850 (BUA 1988) 182 28d, steady-state, 0.003 mg/l, Lepomis macrochirus (Sax 1986) 398 32d, Pimephales promelas (USEPA 1984) 420–1140 6w, Cyprinus carpio, conc 0.05 mg/l, 120–1320 6w, Cyprinus carpio, conc 0.005 mg/l, (MITI 1992)
Bioconcentration factor, crustaceans	142 Daphnia magna, 0.003 mg/l equilibrium (Sax 1986)
Other information about bioaccumulation	Medium level accumulation (Anon. 1989). Confirmed to be accumulated on a medium level (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	756 orl-rat, 300 orl-mus (Lewis & Sweet 1984)
LDLo values to mammals in non-oral exposure, mg/kg	500 ipr-mus (Sax 1986)
Health effects	The amount of TCB necessary to induce a toxic reaction via application to the skin is quite high. 3 to 5 ppm causes minor eye and respiratory irritation. – Severe skin and eye irritation. – CNS stimulation, headache, dermatitis, skin, eye, and throat irritation (Sax 1986). Skin and eye irritation data: skn, rbt, 1950 mg/l, 13 W-I, moderate (Sax 1986).
Carcinogenicity	No carcinogenic effect shown (BUA 1988).
Mutagenicity	Negative in mutagenicity tests (BUA 1988).
Effects on arthropods	LC50, 2 d, 0.93 mg/l, Tanytarsus dissimilis (Holcombe et al. 1987).
Effects on wastewater treatment	BOD test inhibited by > /= 5 mg/l (Sax 1986).

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EC50 values to microorganism, mg/l	280	0.5hr, Resazurin reduction, methanol
	110	0.5hr, Resazurin reduction, ethanol
	50	0.5hr, Resazurin reduction, acetone
	> 500	0.5hr, Resazurin reduction, DMSO (Thompson et al. 1986)
EC50 values to algae, mg/l	8.4	96hr, grw, Scenedesmus subspicatus (Geyer et al. 1985)
	1.4	96hr, growth, Selenastrum capricornutum
	3.9	3hr, photosynthesis, Selenastrum capricornutm (Calamari et al. 1983)
	8.9	Skeletonema, growth (USEPA 1980)
	35.5	96hr, Selenastrum capricornutum chlorophyll destruction
	36.7	96hr, S. capricornutum decreased cell numbers
	8.7	96hr, Skeletonema costatum chlorophyll inhibition
	8.93	96hr, S. costatum decreased cell numbers (Sax 1986)
LC50 values to crustaceans, mg/l	50	48hr, Daphnia magna (LeBlanc 1980)
	0.56	16d, Daphnia magna (Hermens et al. 1984)
	3.02	4d, Orconectes immunis (Holcombe et al. 1987)
	1.2	24hr, Daphnia magna (Calamari et al. 1983)
	2.09	48hr, unfed, Daphnia magna
	1.68	48hr, fed, Daphnia magna (USEPA 1984)
EC50 values to crustaceans, mg/l	0.27	16d, reproduction, Daphnia magna
	0.46	16d, growth, Daphnia (Hermens et al. 1984)
	0.45	14d, rpd, Daphnia magna (Calamari et al. 1983)
	3.39	2d, mbt, Daphnia magna (Holcombe et al. 1987)
	1.7–2.1	48hr, Daphnia magna (Richter et al. 1983)
	3.2	24hr, Artemia (Abernethy et al. 1986)
	2.6	96hr, Nitocra (Bengtsson et al. 1983)
	0.45	96hr, Mysidopsis (USEPA 1980)
	50.2	48hr, Daphnia magna (Sax 1986)
NOEC values to crustaceans, mg/l	0.32	16d, srv, Daphnia magna
	0.1	16d, rpd, Daphnia magna (Hermens et al. 1984)
	0.363–0.694	28d, Daphnia (USEPA 1984)
LC50 values to fishes, mg/l	0.71	48hr, Salmo gairdneri (Calamari et al. 1983)
	2.4	14d, Poecilia reticulata (Könemann 1979)
	2.9	96hr, Pimephales promelas (Veith et al. 1983)
	3.4	96hr, Lepomis macrochirus (Buccafusco et al. 1981)
	21	96hr, Cyprinodon variegatus (Heitmuller et al. 1981)
	3.02	4d, Lepomis macrochirus
	3.01	4d, Pimephales promelas
	1.32	4d, Salmo gairdneri (Holcombe et al. 1987)
	2.76	4d, Pimephales promelas (Carlson 1987)

	1.95	48hr, Salmo gairdneri
	6.3	48hr, Brachydanio rerio (Calamari et al. 1983)
	2.9	96hr, Pimephales (Veith et al. 1983)
	3.4	96hr, Lepomis (Buccafusco et al. 1981)
	0.7	Leuciscus (Knie et al. 1983)
	2.4	7d, Poecilia (Könemann 1981)
	1.5	Salmo gairdneri
	2.87	Pimephales promelas
	3.36	96hr, Lepomis macrochirus
	21.4	96hr, Cyprinodon variegatus (Sax 1986)
	2.76	96hr, flow-through, Pimephales promelas
	1.52	96hr, Salmo gairdneri (USEPA 1984)
	12.3	48hr, Oryzias latipes (MITI 1992)
EC50 values to fishes, mg/l	1.27	96hr, Salmo gairdneri (USEPA 1984)
LOEC values to fishes, mg/l	0.41	30d, Pimephales, embryo-larvae (LeBlanc 1984)
	0.18	21d, Branchydanio (BUA 1988)
NOEC values to fishes, mg/l	0.499–1.008	32d, Pimephales promelas (USEPA 1984)
Other information about water organisms	EC50 (24hr) 0.91 mg/l, rpd, Tetrahymena pyriformis (Yoshioka et al. 1985). Aplexa hypnorum, LC50, 4 d, 3.16 mg/l (Holcombe et al. 1987). 0.286 mg/l; 0.705 mg/l, Pimephales promelas, chronic value, early life stage test. – 0.222 mg/l, Cyprinodon variegatus, chronic value, early life stage test (Sax 1986).	
Other effects on aquatic ecosystems	LOEC, marine model ecosystem: 0.04 mg/l, mollucs being the most sensitive organisms (Tagatz et al. 1985).	
Other information	Theoretical division: 95.7% in air; 1.2% in water; > 3% in sediment and soil (Anon. 1989). Dangerous to environment: not easily degradable; bioaccumulating; toxic to aquatic life (Anon. 1989).	

1935 • 1,3,5-Trichlorobenzene 108-70-3

Synonyms	sym-Trichlorobenzene	
Sumformula of the chemical	$C_6H_3Cl_3$	
Use	Not used directly in any quantity. Used as intermediate in chemical synthesis.	
State and appearance	White crystals; long needles.	
Molecular weight	182	
Vapour pressure, mmHg	0.15	25 °C
	1	78 °C
Water solubility, mg/l	6.59	25 °C (Yalkowsky et al. 1979)
	4.12	25 °C (Miller et al. 1984)
	6.01	25 °C (Banerjee 1984)
Melting point, °C	64	(Suntio et al. 1988)
	63.5	(MITI 1992)
Boiling point, °C	208.5	(MITI 1992)

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Flashing point, °C	107.2
Log octanol/water coefficient, log Pow	4.1 (Anon. 1988) 4.27 (Hansch & Leo 1979) 4.15 (Konemann et al. 1979) 4.2 (Konemann et al. 1979) 4.17 (Wateral et al. 1982) 4.02 (Miller et al. 1984) 4.31 (Chiou 1985) 4.15 (Hawker & Connell 1985)
Log soil sorption coefficient, log Kom	2.85 observed (Sabljic 1987) 2.75 calculated (Sabljic 1987)
Henry's law constant, Pa x m³/mol	1400 (Anon. 1988) 396.9 (Suntio et al. 1988)
Mobility	Equilibrium distribution: *mass %* air 99.40 water 0.20 solid 0.39 (Anon. 1988).
Other physicochemical properties	Can react vigorously with oxidizing materials. Flammability: Moderate fire hazard; nonflammable but gives off combustible fumes. Insoluble.
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30mg/l (MITI 1992).
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Other information about degradation	At 200 mg/l and 30 °C Pseudomonas caused 78% ring disruption in 120 hours (Sax 1986).
Bioconcentration factor, fishes	630-1620 6w, Cyprinus carpio, conc 0.025 mg/l 150-1700 6w, Cyprinus carpio, conc 0.0025 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be accumulated on a medium level (Anon. 1987).
Health effects	The amount of trichlorobenzene necessary to induce a toxic reaction via application to the skin is quite high. Moderately irritating to skin, eyes, and mucous membranes. Moderately hazardous via oral and inhalation routes (Sax 1986).
EC50 values to microorganism, mg/l	320 0.5hr, Resazurin reduction, methanol > 500 0.5hr, Resazurin reduction, ethanol 250 0.5hr, Resazurin reduction, acetone > 500 0.5hr, Resazurin reduction, DMSO (Thompson et al. 1986)
LC50 values to fishes, mg/l	3.3 14d, Poecilia reticulata (Könemann 1979) 12.3 48hr, Oryzias latipes (MITI 1992)
Other information about water organisms	EC50 (24hr) 30 mg/l, rpd, Tetrahymena pyriformis (Yoshioka et al. 1985).

1936 • 2,3,6-Trichlorobenzoic acid 50-31-7

Synonyms	Benzoic acid, 2,3,6-trichloro-
Sumformula of the chemical	C7H3Cl3O2
EINECS-number	2000264
Use	Phytocide.
Water solubility, mg/l	5900 (MITI 1992)
Melting point, °C	60–90 (MITI 1992)
Log octanol/water coefficient, log Pow	0.70–0.97 (MITI 1992)
Total degradation in water	Biodegradation: 0–2% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.4 6w, Cyprinus carpio, conc 0.293 mg/l < 3.5 6w, Cyprinus carpio, conc 0.0293 mg/l (MITI 1992)
Effects on plants	Root segments of aspen (Populus tremula) were treated with buffered solutions of 2,3,6-trichlorobenzoic acid for 24 hours: 0.001 M (concentration of the solution) —strong inhibition of the shoot formation from aspen roots (Eliassaon 1961).
LC50 values to fishes, mg/l	417 48hr, Oryzias latipes (MITI 1992)

1937 • 3,4,4'-Trichlorocarbanilide 101-20-2

Use	Bacteriostate.
Other information about water organisms	LC50 (48hr) 0.032 mg/l, Mercennaria mercennaria (Davis & Hidu 1969).

1938 • 1,1,1-Trichloroethane 71-55-6

Sumformula of the chemical	C2H3Cl3
Use	Solvent; cleaning solvents.
Molecular weight	133
Water solubility, mg/l	4500 20 °C 500–1320 20 °C (Anon. 1986b) 0.44% (MITI 1992)
Melting point, °C	-32 (Suntio et al. 1988)
Boiling point, °C	74 (Anon. 1986b) 74 (MITI 1992)
Log octanol/water coefficient, log Pow	2.49 (Anon. 1986)b 2.95 (Anon. 1988) 2.17 (Schwarzenbach et al. 1983) 2.49 (Hansch & Leo 1979) 2.47 (Banerjee et al. 1980)

ST

Henry's law constant, Pa x m³/mol

13000	(Anon. 1988)
2800	exptl. (Dilling 1977)
1743	exptl. (Gossett 1987)

Volatilization

Relative volatility (nBuAc=1) = 7.50

Mobility

Equilibrium distribution:

	mass %
air	99.98
water	0.02
solid	0.00

(Anon. 1988)

Total degradation in water

Biodegradation:
0% by BOD
period: 14d
substance: 100 mg/l
sludge: 30 mg/l
(MITI 1992)

Other information about degradation

Degradation of 1,1,1-trichloroethane:

ENVIRONMENT	*INIT mg/l*	*REDOX-COND.*	*TEMP. °C*	*DEGRADATION %/day*	*t1/2*	*REF.*
biofilm	0.017	methanogen	22	-	15 (1)	a
biofilm	0.016	aerobic	22	0/730	-	b
water	0.229	methanogen	35	85/16	6	c
water	0.053	denitrif.	25	0/56	> 56	d
biofilm	0.17	denitrif.	23	-	3466 (1)	e
biofilm	0.17	sulfate red.	23	-	1386 (1)	e
biofilm	0.17	methanogen	23	-	7 (1)	e
water (deion.)	1.0	aerobic	25	-	180	f
soil	0.21	aerobic + natural gas		-	0.43	g
water (adapted)	0.171	aerobic		97/11	-	h
water (adapted)	5	aerobic	25	29/7	-	i
water	10	aerobic	25	23/7	-	i
water	5	aerobic	25	83/7	2.7	i
water	10	aerobic	25	75/7	3.5	i
groundwater	1.8	aerobic	20	-	> 1022	j
soil	0.765	aerobic + propane		0/25	-	k
soil	0.6–0.8	aerobic	17	< 3/7	-	l

(1) Biomass concentration set to 0.100 mg/l.

a) Bouwer & McCarty 1985
b) Bouwer & McCarty 1982
c) Bouwer & McCarty 1983a
d) Bouwer & McCarty 1983b
e) Bouwer & Wright 1987
f) Dilling et al. 1975
g) Anon. 1987b
h) Kästner 1986
i) Tabak et al. 1981
j) Vogel & McCarty 1987
k) Wilson & White 1986
l) Wilson et al. 1983

Bioconcentration factor, fishes

9	28 d, Lepomis macrochirus (Anon. 1986)b
0.7–3.0	6w, Cyprinus carpio, conc 0.3 mg/l
0.9–4.9	6w, Cyprinus carpio, conc 0.03 mg/l
	(MITI 1992)

Other information about bioaccumulation

Confirmed to be non-accumulative or low accumulative (Anon. 1987).

LD50 values to mammals in oral exposure, mg/kg

750 orl-dog

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Maximum longterm immission concentration in air for plants, mg/m³	30	VDI 2306
Maximum longterm immission concentration in air for plants, ppm	5	VDI 2306
Effects on microorganisms	LC50, Photobacterium phosphoreum, 18,2 mg/l, 5 min LC50, Photobacterium phosphoreum, 8,0 mg/l, 5min (Anon. 1986b)	
EC50 values to algae, mg/l	320 > 669	24hr, assimulations test mg/l, 96hr, Selenastrum capricornutum, cellnumber and chlorophyll a (Anon. 1986b)
LC50 values to crustaceans, mg/l	> 530 530	48hr, Daphnia magna (LeBlanc 1980) 48hr, Daphia magna (Anon. 1986b)
LC50 values to fishes, mg/l	53 133 72 71 123 105 52.8 69.7 73	96hr, Pimephales promelas, 7d, Poecilia reticulata (Könemann 1979) 96hr, Lepomis macrochirus (Buccafusco et al. 1981) 96hr, Cyprinodon variegarus (Heitmuller et al. 1981) 48hr, Leuciscus idus melantus Pimephales promelas Pimephales promelas 96hr, Lepomis macrochirus (Anon. 1986b) 48hr, Oryzias latipes (MITI 1992)

1939 • 1,1,2-Trichloroethane 79-00-5

Synonyms	Vinyltrichloride	
Use	Manufacturing of 1,1-dichloroethylene; solvent for chlorinated rubber and various organic materials (fats, oils, resins). Intermediate.	
State and appearance	Colourless liquid.	
Molecular weight	133.4	
Vapour pressure, mmHg	19	20 °C
Water solubility, mg/l	4500 < 10 mg/l	0 °C (MITI 1992)
Melting point, °C	-35.5	(MITI 1992)
Boiling point, °C	113.7	
Log octanol/water coefficient, log Pow	2.13	(Anon. 1988)
Log soil sorption coefficient, log Kom	1.87 1.7	observed (Sabljic 1987) calculated (Sabljic 1987)
Henry's law constant, Pa x m³/mol	74 97.34	(Anon. 1988) calc. (Yaws et al. 1991)
Volatilization	Relative volatility (nBuAc=1) = 7.5	

ST

Mobility	Equilibrium distribution: *mass %* air 96.16 water 3.76 solid 0.08 (Anon. 1988)
Total degradation in water	Biodegradation: 5% by GC analysis period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992)
Bioconcentration factor, fishes	0.7–2.6 6w, Cyprinus carpio, conc 0.3 mg/l 2.7–6.7 6w, Cyprinus carpio, conc 0.03 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	580 orl-rat (Lewis & Sweet 1984) 100–200 orl-rat (Verschueren 1983) 1140 orl-rat
LD50 values to mammals in non-oral exposure, mg/kg	3730 skn-rbt (Lewis & Sweet 1984)
LDLo values to mammals in oral exposure, mg/kg	500 orl-dog (Lewis & Sweet 1984)
LCLo values to mammals in inhalation exposure, ppm	500 8hr, ihl-rat (Lewis & Sweet 1984)
Carcinogenicity	NCI carcinogenesis bioassay completed: results positive, mus; results negative, rat (Lewis & Sweet 1984)
LOEC values to algae, mg/l	430 rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980)a
LC50 values to crustaceans, mg/l	18 48hr, Daphnia magna (LeBlanc 1980) 186 48hr, unfed, Daphnia magna 174 48hr, fed, Daphnia magna (USEPA 1984)
EC50 values to crustaceans, mg/l	80.6 48hr, unfed, Daphnia magna 77.8 48hr, fed, Daphnia magna (USEPA 1984)
NOEC values to crustaceans, mg/l	13.2–26.0 28d, Daphnia (USEPA 1984)
LC50 values to fishes, mg/l	40 96hr, Lepomis macrochirus (Buccafusco et al. 1981) 94 7d, Poecilia reticulata (Könemann 1979) 82 96hr, Pimephales promelas (Veith et al. 1983) 81.6 96hr, flow-through, Pimephales promelas (USEPA 1984) 133 48hr, Oryzias latipes (MITI 1992)
NOEC values to fishes, mg/l	6.0–14.8 32d, Pimephales promelas (USEPA 1984)

1940 • 2,2,2-Trichloroethanol 115-20-8

EC50 values to microorganism, mg/l	44 Microtox (Nacci et al. 1986)
LC50 values to fishes, mg/l	299 96hr, Pimephales promelas (Veith et al. 1983)

ST

1941 • Trichloroethylene

79-01-6

Synonyms	Trichloroethene Acetylene trichloride Ethylene trichloride Trilene TCE 1,1,2-Trichloroethylene
Sumformula of the chemical	C2HCl3
Purity, %	> 98%
Known impurities	Amines * as stabilizers 0.001–0.01%* Combinations of epoxides * and esters * 0.2–2.0% total (Fawell & Hunt 1988).
Use	Solvent used for degreasing metals and as a dry-cleaning agent. It has been used as an anaesthetic by inhalation, although this use is now infrequent. Solvent in food processing.
Odour	Odour threshold: 10 mg/l in water (Verschueren 1983).
Molecular weight	131.38
Water solubility, mg/l	1000–1100 20 °C (Anon. 1986b) 1100 25 °C (Anon. 1986b) > 500 (MITI 1992)
Melting point, °C	-73 (Suntio et al. 1988) -73 (MITI 1992)
Boiling point, °C	86.9 (Anon. 1986b) 87.2 (MITI 1992)
Log octanol/water coefficient, log Pow	2.42 (Anon. 1986) 2.29–3.30 (Sabljic 1987) 2.29 (Anon. 1986b) 2.53 (Anon. 1988) 2.29 (Schwarzenbach et al. 1983) 2.42 (Banerjee et al. 1980)
Log soil sorption coefficient, log Kom	2 observed (Sabljic 1987) 1.7 calculated (Sabljic 1987)
Henry's law constant, Pa x m³/mol	1101 calc. (Gossett 1987) 971 exptl. (Gossett 1987) 1182 calc. (Yaws et al. 1991)
Volatilization	Relative volatility (nBuAc=1) = 6.99
Mobility	28.65% (air), 71.27% (water), 0.08% (sediment). Equilibrium distribution: *mass %* air 99.67 water 0.31 solid 0.02 (Anon. 1988).
Total degradation in water	Biodegradation: 2.4% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

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Other information about degradation

Degradation of trichloroethylene:

ENVIRONMENT	*INIT. mg/l*	*REDOX-COND.*	*TEMP. °C*	*DEGRADATION %/day*	*t1/2*	*REF.*
soil	5	anaerobic	25	-	33-90	a
aquifer material	0.085	anaerobic	20	< 3/7	-	b
water (mixed cult.)	0.012	methanogen	35	25/112	270	c
water	0.034	methanogen	35	12/112	620	c
water	0.127	methanogen	35	46/112	127	c
water	0.011	aerobic	20	0/175	> 175	c
water	0.031	aerobic	20	0/175	> 175	c
water	0.081	aerobic	20	0/175	> 175	c
water	0.178	methanogen	35	40/57	78	d
water (deion.)	1.0	aerobic	25	-	320	e
water	0.08	aerobic+methane	20	81/0.3	< 2	f
water	0.65	aerobic	20	69/4	2.4	f
soil	1.0	aerobic+natural gas		-	0.03	g
water (adapted)	1.436	aerobic	-	97/11	-	h
water	50	aerobic	-	44/14	-	h
water	36	aerobic/anaerobic		56/16	-	h
water	5	aerobic	25	64/7	-	i
water	10	aerobic	25	38/7	-	i
water (adapted)	5	aerobic	25	86/7	-	i
water	10	aerobic	25	84/7	-	i
soil	0.82	aerobic + propane		-	5-9	j
soil	0.9	aerobic	20	14/2	-	k
soil	0.18	aerobic	20	0/2	-	k
aquifer material	0.6–0.8	aerobic	17	< 2/7	< 1.2	l
soil	0.15	aerobic + methane		95/7	-	m

a) Barrio-Lage et al. 1987
b) Wilson et al. 1983b
c) Bouwer et al. 1981
d) Bouwer & McCarty 1983a
e) Dilling et al. 1975
f) Fogel et al. 1986
g) Anon. 1987b
h) Kästner 1986 (1000000000 org./ml)
i) Tabak et al. 1981
j) Wilson & White 1986
k) Wilson et al. 1981
l) Wilson et al. 1983
m) Wilson & Wilson 1985
(Anon. 1987b).

Metabolism in mammals

Trichloroethylene is absorbed into the body through the lungs, gastrointestinal tract and the skin. Following oral administration of 5, 10 and 25 mg/kg to male rats, trichloroethylene appeared rapidly in the blood, with concentrations peaking after 6–10 min. This compound is easily absorbed across the gastrointestinal tract in man, and many cases of acute poisoning following oral ingestion have been reported (Fawell & Hunt 1988).

Trichloroethylene is absorbed through the skin in man, although the significance of this route of exposure for dilute aqueous solutions is still unclear (Fawell & Hunt 1988).

Trichloroethylene is distributed primarily to the adipose tissue, due to its high fat solubility (Fawell & Hunt 1988).

Transplacental diffusion has been demonstrated in humans, and trichloroethylene was detected in foetal blood (Fawell & Hunt 1988).

This compound is readily metabolized by rodents, primates and man. In the liver, metabolic breakdown of trichloroethylene is thought to involve transformation by mixed function oxidase enzymes to a reactive epoxide. The instability of this epoxide has been attributed to its non-symmetrical arrangement of chlorine atoms. A rearrangement of the epoxide results in the formation of chloral. This may be either oxidized to trichloroacetic acid, or reduced to trichloroethanol.

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	Trichloroethanol products may also be conjugated to form glucoronides. The identification of HAAE (N-(hydroxyacetyl)-aminoethanol) and oxalic acid in the urine of rats and mice after a single oral dose of radiolabelled trichloroethylene indicates that dechlorination reactions may also occur in the breakdown of this compound. However, in man the principal metabolites following absorption of trichloroethylene appear to be trichloroacetic acid and trichloroethanol (Fawell & Hunt 1988). Recent studies suggest that trichloroethylene may also be metabolized to some extent in the kidney, to form a cysteine conjugate. The production of reactive intermediated during this process may explain the nephrotoxicity and nephrocarcinogenicity of trichloroethylene observed in rats (Fawell & Hunt 1988). Trichloroethylene metabolism appears to be a dose-dependent process in rats and man (Fawell & Hunt 1988).
Other information about metabolism	Alcohol in the blood inhibits metabolism of this compound and may cause 'Degreaser's flush'. Symptoms include drowsiness and reddening of the face and upper body (Fawell & Hunt 1988). The major route of elimination is via the lungs. The rest is eliminated in the urine. Following metabolism of trichloroethylene, the elimination of various metabolites in the urine occurs at different rates. The slower excretion rate of trichloroacetic acid compared to trichloroethanol may be due to its higher affinity for proteins (Fawell & Hunt 1988).
Bioconcentration factor, fishes	17 — 14d, Lepomis macrochirus 19 — 14d, Brachydanio rerio 15 — 8d, Brachydanio rerio (Anon. 1986b) 4.3–17.0 — 6w, Cyprinus carpio, conc 70 000 mg/l 4.0–16.0 — 6w, Cyprinus carpio, conc 7000 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1984).
LD50 values to mammals in oral exposure, mg/kg	4920 — orl-rat (Torkelson & Rowe 1982) 2443 — orl-mus, female 2402 — orl-mus, male (Tucker et al. 1982) 7200 — orl-rat, 14d 4421 — orl-rat, 14d, 4421/6802 mg/kg 6802 — orl-rat, 14d (Anon. 1986b)
Effects on the reproduction of mammals	Trichloroethylene appears to be of low reproductive toxicity. There were no significant effects on fertility, teratogenicity or neonatal development in rodents. Delayed ossification of the sternum and displacement of the right ovary were observed in the offsping of treated Long-Evans rats, but these do not represent important embryotoxic effects (Schwetz et al. 1975, Dorfmueller et al. 1979, Taylor et al. 1985, Ghantous et al. 1986, Manson et al. 1984, Zenick et al. 1984, Borzelleca & Carchman 1982, Fawell & Hunt 1988).
Other information about mammals	The toxicology of trichloroethylene has been well studied and it appears to be of low acute and chronic toxicity. The principal target organs are the CNS and liver, although recent evidence suggests that trichloroethylene may be nephrotoxic in rodents following long-term exposure (Fawell & Hunt 1988, Tucker et al. 1982, Torkelson & Rowe 1982, Adams et al. 1951, Kjellstrand et al. 1982, Kanje et al. 1981, Stott et al. 1982, Kjellstrand et al. 1981, Aranyi et al. 1986, Sanders et al. 1982, WHO 1985, Feldman et al. 1985, Vernon & Ferguson 1969, James, 1963, Hayden et al. 1976, Wells 1982, Buben & O'Flaherty 1985, US NTP 1983, Kyrklund et al. 1983, Silverman & Williams 1975, Mitchell & Parsons-Smith 1969, Barret et al. 1982, Vyskocil 1953).

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Carcinogenicity	In 1976 the National Cancer Institute study found an increase in liver tumours in C6B3F1 mice following chronic oral exposure to trichloroethylene. An increase in forestomach tumours in Swiss mice and lung tumours in NMRI mice from oral and inhalation exposure have also been reported. The carcinogenic potential of trichloroethylene appears to be affected by the presence of stabilisers. There was no evidence of hepatocarcinogenicity in Osborne-Mendel rats. However, a number of renal adenocarcinomas have been recently reported in rats following long-term oral administration, which are rare in untreated controls. Epidemiology studies are insufficient to assess whether trichloroethylene causes cancer in man (WHO 1985, Dekant et al. 1986a, Henschler et al. 1984, Fukuda et al., Henschler et al. 1980, Van Duuren et al. 1983, Tu et al. 1985, Blair et al. 1979, Tola et al. 1980, Paddle 1983, Fawell & Hunt 1988).
Mutagenicity	There is conflicting evidence that trichloroethylene is mutagenic. Both positive and negative results were reported in the Ames test with and without metabolic activation. Trichloroethylene does no appear to be mutagenic in yeast in the absence of metabolic activation, but the position is unclear in the presence of S-9. Under certain conditions of growth, trichloroethylene disrupts mitotic segregation in the fungus Aspergillus nidulans. Unscheduled DNA synthesis and chromosome aberrations were reported in human lymphocytes following exposure to this compound. The metabolite S-1,2-dichlorovinylcysteine was mutagenic in the Ames test without metabolic activation. The differences in mutagenicity observed in these studies may be partly explained by the purity and nature of the additives present in the samples tested. Both epichlorohydrin and epoxybutane, two stabilizers found in technical grade trichloroethylene, were mutagenic in vitro. At present, there are inadequate data to evaluate the mutagenic potential of this chemical (Waskell 1978, Bartsch et al. 1979, Cerna & Kypenova, Greim et al. 1975, Bronzetti et al. 1978, Callen et al. 1980, Rossi et al. 1983, Crebelli et al. 1985, Slacik-Erben et al. 1980, Bergman 1983, Walles 1986, Perocco & Prodi 1981, Konietzko et al. 1978, Dekant et al. 1986b).
Effects on invertebrates	EC50, Eisenia foetida, 1000 mg/kg, 28d (Anon. 1986b)
Effects on plants	EC50, Brassica rapa sativa rapifera, 1000 mg/kg, 14d; EC50, Avena sativa, 1000 mg/kg, 14d (Anon. 1986b)
Maximum longterm immission concentration in air for plants, mg/m³	30 VDI 2306
Maximum longterm immission concentration in air for plants, ppm	5 VDI 2306
Effects on microorganisms	EC50, Photobacterium phosphoreum, 115 mg/l, 15 min; EC50, assimilationtest, 530 mg/l, 24hr. (Anon. 1986b). Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 65 mg/l (Bringmann & Kühn 1980a).
EC50 values to algae, mg/l	450 96hr, grw, Scenedesmus subspicatus (Geyer et al. 1985) 450 4d, Scenedesmus subspicatus (Anon. 1986b)
LOEC values to algae, mg/l	63 rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
NOEC values to algae, mg/l	175 rpd, schr, Selenastrum capricornutum (Slooff et al. 1983)

LC50 values to crustaceans, mg/l	18	48hr, Daphnia magna (LeBlanc 1980)
	65	48hr, Daphnia magna
	45	48hr, Daphnia pulex
	57	48hr, Daphnia cucullata (Canton & Adema 1978)
	85.2	48hr, Daphnia magna
	100	Daphnia magna
	94	Daphnia magna
	41	Daphnia magna
	43	Daphnia magna
	56	Daphnia magna
	51	Daphnia pulex
	39	Daphnia pulex (Anon. 1986b)
	30	48hr, Asellus aquaticus (Slooff 1983)
	24	48hr, Gammarus pulex (Slooff 1983)
EC50 values to crustaceans, mg/l	1313	24hr, Daphnia magna (Anon. 1986b)
LC50 values to fishes, mg/l	41	96hr, Pimephales promelas
	55	7d, Poecilia reticulata (Könemann 1979)
	42	48hr, Salmo gairdneri (Slooff et al. 1983)
	45	96hr, Lepomis macrochirus (Buccafusco et al. 1981)
	44	96hr, Pimephales promelas (Veith et al. 1983)
	136/203	mg/l, 48hr, Leuciscus idus melanotus
	40.7	96hr, Pimephales promelas
	66.8	96hr, Pimephales promelas
	44.7	96hr, Lemomis macrochirus (Anon. 1986b)
	45	96hr, flow-through, Pimephales promelas (USEPA 1984)
	59	48hr, Oryzias latipes (MITI 1992)
EC50 values to fishes, mg/l	21.9	96hr, Pimephales promelas (Anon. 1986b)
Other information about water organisms		EC50 (24hr) 410 mg/l, rpd, Tetrahymena pyriformis (Yoshioka et al. 1985). LC50, 48hr, 132 mg/l, Tubificidae LC50, 48hr, 64 mg/l, Chironomus gr. thummi LC50, 48hr, 75 mg/l, Erpobdella octoculata LC50, 48hr, 56 mg/l, Lymnaea stagnalis LC50, 48hr, 42 mg/l, Dugesia cf. lugubris LC50, 48hr, 75 mg/l, Hydra oligactis LC50, 48hr, 110 mg/l, Corixa punctata LC50, 48hr, 49 mg/l, Ischura elegans LC50, 48hr, 70 mg/l, Nemoura cinerea LC50, 48hr, 42 mg/l, Cloeon dipterum (Slooff 1983) Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): > 1000 mg/l protozoa (Entosiphon sulcatum): 1200 mg/l (Bringmann & Kühn 1980a)

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Other information	Atmosperic contamination with trichloroethylene has been implicated as a possible factor in the depletion of the ozone layer (Fawell & Hunt 1988). since trichloroethylene is virtually insoluble in water, and has a specific gravity heaviere then water, any pollution of groundwater is likely to persist. There is no indication that trichloroethylene is produced from chlorination of natural waters (Fawell & Hunt 1988).

1942 • Trichloroethylphosphate 306-52-5

LC50 values to fishes, mg/l	210 90	96hr, Oryzias latipes 96hr, Carassius auratus (Sasaki et al. 1981)
Other information about water organisms	EC50 (24hr) 91 mg/l, rpd, Tetrahymena pyriformis (Yoshioka et al. 1985).	

1943 • Trichlorofluoromethane 75-69-4

Use	Blowing agent; aerosols.	
Molecular weight	137	
Log octanol/water coefficient, log Pow	2.4	(Anon. 1988)
Henry's law constant, Pa x m³/mol	11000 12340	(Anon. 1988) calc. (Yaws et al. 1991)
Mobility	Equilibrium distribution: air water solid	 *mass %* 99.97 0.03 0.00 (Anon. 1988).

1944 • 3,4,5-Trichloroguaiacol 57057-83-7

Sumformula of the chemical	C7H502Cl3	
Molecular weight	227.49	
Log octanol/water coefficient, log Pow	4.145	(Xie 1984)
LC50 values to algae, mg/l	0.8	96hr, Selenastrum capricornutum (Kuivasniemi et al. 1985)
LC50 values to fishes, mg/l	0.75	96hr, Salmo gairdneri (Leach & Thakore 1975, Voss et al. 1980)

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1945 • 4,5,6-Trichloroguaiacol 2668-24-8

Sumformula of the chemical	C7H502Cl3	
Molecular weight	227.49	
pKa	7.2	
Log octanol/water coefficient, log Pow	3.83	(Xie 1984)

1946 • 1,3,5-Trichloroisocyanuric acid 87-90-1

Sumformula of the chemical	C3Cl3N3O3
EINECS-number	2017828
Total degradation in water	Biodegradation: 0% by BOD (dechlorinated to isocyanuric acid) period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).

1947 • 2,4,5-Trichloronitrobenzene 89-69-0

Synonyms	1,2,4-Trichloro-5-nitrobenzene	
LD50 values to birds in oral exposure, mg/kg	100 > 100	orl-Agelaius phoeniceus orl-Sturnus vulgaris (Schafer et al. 1983)
EC50 values to microorganism, mg/l	8 0.7	Microtox (Kaiser and Ribo 1985) Microtox (Kaiser and Ribo 1985)

1948 • 2,4,6-Trichloronitrobenzene 18708-70-8

Sumformula of the chemical	C6H2O2NCl3	
Water solubility, mg/l	6.25	(MITI 1992)
Melting point, °C	72	(MITI 1992)
Log octanol/water coefficient, log Pow	3.32	(MITI 1992)
Bioconcentration factor, fishes	123–464 137–372	8w, Cyprinus carpio, conc 0.01 mg/l 8w, Cyprinus carpio, conc 0.001 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non–accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	5.3	48hr, Oryzias latipes (MITI 1992)

1949 • Trichloronitromethane 76-06-2

Sumformula of the chemical	CCl3NO2	
Use	Organic synthesis; dye-stuffs; fumigants; fungicides; insecticides; rat exterminator; poison gas.	
Odour	Odour: T.O.C.: 1.1 ppm (7.3 mg/m³ = 1.09 ppm)	
Molecular weight	164.39	
Specific gravity (water=1)	1.651	at 20/4 °C
Conversion factor, 1 ppm in air=	6.72	
Conversion factor, 1 mg/m³ in air=	0.149	

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Vapour pressure, mmHg	16.9 33	20 °C 30 °C
Water solubility, mg/l	2000	
Melting point, °C	-64	
Boiling point, °C	112	
Volatilization	Sat.conc.	170 g/m³ at 20 °C 286 g/m³ at 30 °C
LD50 values to mammals in oral exposure, mg/kg	250	orl-rat (Verschueren 1983)
LC50 values to mammals in inhalation exposure, ppm	117–140	1ppm LC43 30min ihl-dog (Patty 1967)
Health effects	Man:	lowest irritant conc.: 1.3 ppm intolerable: 7.5 ppm, 10 min 15.0 ppm, 1 min lethal: 119 ppm, 30 min 297 ppm, 10 min (Patty 1967).
Carcinogenicity	The bioassay of chloropicrin using Osborne-Mendel rats did not permit an evaluation of carcinogenicity because of the short survival time of dosed animals. The bioassay of chloropicrin using B6C3F1 mice did not provide conclusive statistical evidence for the carcinogenicity of this compound (Verschueren 1983).	

1950 • Trichlorophenol 25167-82-2

Sumformula of the chemical	C6H3OCl3	
Water solubility, mg/l	< 1000	(MITI 1992)
Melting point, °C	69	(MITI 1992)
Boiling point, °C	246	(MITI 1992)
Total degradation in water	Biodegradation: 82.5% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

1951 • 2,3,5-Trichlorophenol 933-78-8

LC50 values to fishes, mg/l	1.6	24hr, Poecilia reticulata (Könemann 1979)

1952 • 2,3,6-Trichlorophenol 933-75-5

Sumformula of the chemical	C6H3OCl3	
Molecular weight	197.45	
Water solubility, mg/l	450	(Cheung 1984)
Melting point, °C	58	(Suntio et al. 1988)
pKa	7.13	(Doedens 1967)
Log octanol/water coefficient, log Pow	3.6	(Xie 1984)

LC50 values to fishes, mg/l	5.1 24hr, Poecilia reticulata (Könemann 1979)

1953 • 2,4,5-Trichlorophenol

95-95-4

Synonyms	Dowicide 2 Phenachlor	
Sumformula of the chemical	C6H3Cl3O	
Purity, %	95	technical grade
Known impurities	* Sometimes at levels 0.07–6.2 ppm: 2,3,7,8-tetrachlorodibenzo-p-dioxin2,7-dichlorodibenzo-p-dioxin 1,3,6,8-tetrachlorodibenzo-p-dioxinpentachlorodibenzo-p-dioxin	
Use	Feedstock in the synthesis of various herbicides. Used in cooling towers, paper and pulp mill systems, hide and leather processing, and disinfection. Minor use as a fungicide in polyvinyl acetate emulsions. Used as adhesives and as a rubber additive. Bactericide. Starting material in manufacture of a series of industrial and agricultural chemicals; 2,4,5-T production; textile industry. Used in manufacture of the pesticides silvex, ronnel and sodium 2,4,5-trichlorophenate. Used on swimming pool related surfaces; household sickroom equipment; food processing plants and equipment; food contact surfaces; hospital rooms; sickroom equipment and bathrooms.	
State and appearance	Solid, grey flakes (sink in water).	
Odour	Phenolic. Odour threshold: water, 0.0112 mg/l; 0.011–0.333 mg/l; taste threshold: water, 0.0017 (lower) (Sax 1986).	
Molecular weight	197.44	
Specific gravity (water=1)	1.678	
Vapour pressure, mmHg	400 1	225 °C 72 °C
Water solubility, mg/l	1190 948 982 100	25 °C 25 °C, pH 5.1 (Blackman et al. 1955) 25 °C (Cheung 1984) (MITI 1992)
Melting point, °C	67	(MITI 1992)
Boiling point, °C	253	(MITI 1992)
pKa	6.74 7.43	(Sax 1986) (Doedens 1967)
Log octanol/water coefficient, log Pow	3.72 3.70–4.19 3.72 3.72	(Sax 1986) (Sabljic 1987) (Hansch & Leo 1979) (Mackay 1982)
Log soil sorption coefficient, log Kom	3.36 2.99	observed (Sabljic 1987) calculated (Sabljic 1987)
Henry's law constant, Pa x m³/mol	0.1887	calc. (Suntio et al. 1988)
Adsorption/desorption	Sorption of 2,4,5-TCP by Bentone 24 (Wyoming bentonite coated with dimethylbenzyl octadecylamine chloride) and Bentone 18C (Wyoming bentonite with sorbed dodecylamine), both organo-clays, was studied. Sorption was accomplished from solution at 20 °C +/- 1 °C during 45 to 48 hour constant shaking period in darkened rooms. The 2,4,5-TCP concentration was 0.5 mM with 5 g Bentone in a 0.005 M KCHO3 buffer. pH's examined were 7.6 (pKa = 7.74, 82% proto lysis) and 7.4 (29% proto lysis). Analysis was via UV-techniques. At pH 7.6 on Bentone 24, 97.8% of the initial amount was sorbed and at pH 7.4, on Bentone 18C, 63.6% of the initial amount was sorbed (Sax 1986).	

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	Soluble in alcohol, ether and acetone. Solubility (g/100g solvent) at 25 °C: 615 acetone; 163 benzene; 51 carbon tetrachloride; 525 diethyl ether; 525 denatured alcohol; 615 methanol; 56 liquid petrolatum (50 °C); 79 soya bean oil; 122 toluene (Sax 1986).
Photochemical degradation in water	2,4,5-TCP was shown to be a major photolytic product of 2,4,5-T when it was exposed to UV radiation in aqueous solution. The rate of photolysis to 2,4,5-TCP was slow, however, the rate of photolysis of 2,4,5-TCP was rapid. The suggested pathway of degradation of 2,4,5-TCP was to 2,5-dichlorophenol or 2,4-dichlororesorcinol, either of which may go to 4-chlororesorcinol and eventually to humic acid polymers. Experimental conditions were as follows: 100 mg/l 2,4,5-T in distilled H2O, pH 8.0 (adjusted with 0.1 N NaOH), irradiation was by summer sunlight in Davis, CA. or UV light (300–450 nm) with light intensity measured at 3.9mW/cm² in the center of the 3 l sample flask and 0.785 mW/cm² halfway from the center to the lamp surface, temperature was 30 °C and filtered air was passed through the solution to maintain saturation. Indoor irradiation was for 200 hours and outdoor exposure was about 9 hours each day for 60 days (540hr). Analysis of samples was by GLC-thermal conductivity detector and isolated products were identified by IR spctra (KBr-disks) and MS (Sax 1986).
Aerobic degradation in soil	AEROBIC DEGRADATION IN SOIL Maximum adsorption wavelength: 291 nm NON-STERILE SOIL Minimum time for > 70% decrease: 80.0–160.0 d % decomposition at the termination of the experiment: 160d, 72% STERILE SOIL % decomposition at the termination of the experiment: 160d, 9% (Baker et al. 1980)
Anaerobic degradation in soil	ANAEROBIC DEGRADATION IN SOIL Maximum adsorption wavelength: 291 nm NON-STERILE SOIL % decomposition at the termination of the experiment: 80d, 8% STERILE SOIL % decomposition at the termination of the experiment: 80d, 5% (Baker et al. 1980)
Total degradation in soil	Decomposition in suspended soils: > 72 days for complete disappearance (Verschueren 1983). There is evidence that 2,4,5-TCP is a metabolite or primary degradation product of a number of pesticides including 2,4,5-T, Silvex, Ronnel, lindane and benzene hexachloride. – 2,4,5-TCP, a metabolite of 2,4,5-T, was converted by microorganisms in the soil suspensions to products that were identified as 3,5-dichlorocatechol, 4-chlorocatechol and succinate by gas chromatography and mass spectrometry, and to products that were tentatively identified as cis, cis-2,4-dichloromuconate, 2-chloro-4-(carboxymethylene)but-2-enolide and chlorosuccinate by gas chromatography and TLC. Microbial decomposition in soils was studied using the shake culture method. The medium was as follows: 0.5 g ammonium sulfate, 0.03 g ferrous sulfate, 0.2 g magnesium sulfate, 0.2 g monobasic and 0.8 g dibasic potassium phosphate and 0.1 g calcium chloride in 1000 ml distilled H2O. The medium was sterilized and had a pH of 7.2. 2,4,5-TCP was added to a final concentration of 0.050 mg/ml and 4 g of freshly sampled soil was added to 100 ml of medium as an inoculum. Temperature was 30 °C, and cultured were aerated on the shaker. Two types of soils were used: Mardin silt loam and Dunkirk silt loam. UV spectrosphotometry was used to measure persistence. Days for complete disappearance in Dunkirk and Mardin soils was 72 + and 47 + days, respectively. Both tests showed persistence for the duration of the incubation (Sax 1986).

Total degradation in water	Took 35 days to obtain 70% degradation of 1 ppm in a batch experiment with mineral water; no degradation at all in seawater (Sax 1986). Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992). The persistence of 2,4,5-TCP was studied in aeration lagoon effluents. The initial concentration of 2,4,5-TCP was 18.8 mg/l. pH of the acid-phenol mixture was adjusted to 7.0 just prior to mixing with the effluent and the system was maintained at 20–21 °C. Complete degradation was noted within 7 days (Sax 1986).
Other information about degradation	The theoretical oxygen demand data showed 44% of 2,4,5-trichlorophenol sample had been degraded in 5 days, and 75% in 20 days. Others report it resistant to microbial decomposition (Sax 1986). Degradation of 2,4,5-trichlorophenol:

ENVIRONMENT	*INIT.CONC. mg/l*	*REDOX-COND.*	*TEMP. °C*	*DEGRADATION %/day*	*REF.*
water (PCP-ad.)	–	aerobic	–	0/1	a
groundwater	60–100	sulfate reducing	room	52/90	b
groundwater	60–100	methanogen	room	39/90	b
lake sediment	60–100	anaerobic	room	100/90	b
active sludge	60–100	anaerobic	37	32/90	b
soil suspension	10–100	aerobic	30	100/72	c
soil suspension	10–100	aerobic	30	100/47	c
soil	1	aerobic	23	72/160	d
sterile soil	1	aerobic	23	9/160	d
soil	1	anaerobic	23	8/80	d
sterile soil	1	aerobic	23	5/80	d

a) Steiert & Crawford 1985 b) Gibson & Suflita 1986
c) Alexander & Aleem 1961 d) Baker & Mayfield 1980
(Anon. 1987b).

Metabolism in mammals	2,4,5-TCP was not found in significant levels in the feces or in detectable quantities in the urine following oral administration of 1 mg/kg to 8 humans. – 2,4,5-TCP is a metabolite of α hexachlorocyclohexane in rat urine. – There was no significant percutaneous absorption of 2,4,5-TCP on the intact skin of rabbits or guinea pigs. – The 2,4,5-trichlorophenol derived herbicides, 2,4,5-T and Silvex, were fed at low dose levels of 0, 300, 1000, and 2000 mg/kg diet to adult cattle and sheep for 28 days. Tissues were sampled 1 day and 1 week after the last dose was given. No residues of 2,4,5-T were found in the fat of sheep receiving 2000 mg/kg diet. Average residue levels in liver were over 6 times the average in kidney: 6.1 vs 0.90, and 4.4 vs 0.81 mg/kg in tissues taken 1 day and 7 days after treatment, respectively. Muscle and fat of sheep and cattle fed Silvex contained no detectable levels of 2,4,5-TCP residues. Levels were slighly higher in liver (0.60–0.63 mg/kg) than in kidney (< 0.05–0.17 mg/kg). – Cows were fed rations containing 2,4,5-T and Silvex at six levels (10–1000 mg/kg diet) for 2 or 3 weeks. Milk and cream samples were collected at various intervals during the feeding of the chemicals and during the 7 days following withdrawal of the highest level. No residue of 2,4,5-T greater than 0.05 mg/kg was found in milk or cream from those fed 10–30 mg/kg diet levels. With 1000 mg/kg diet, avetage residues were 0.23 mg/kg 2,4,5-TCP in milk and 0.19 mg/kg in cream. No residues of 2,4,5-TCP were found in any of the samples of milk or cream from cows fed Silvex (Sax 1986).
Bioconcentration factor, fishes	62 Carassius auratus (Verschueren 1983) 121–484 8w, Cyprinus carpio, conc 0.01 mg/l 232–825 8w, Cyprinus carpio, conc 0.001 mg/l (MITI 1992)

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Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987). Half-life in the blood of sheep approximately 20hr. – The concentration ration for goldfish in 1 ppm for 12hr was approximately 45. No elimination rates in clean water were determined (Sax 1986).	
LD50 values to mammals in oral exposure, mg/kg	820 600 4000 2960 2800 3000 1000	orl-rat orl-mus (Lewis & Sweet 1984) orl-rat orl-rat orl-rat orl-rat orl-gpg (Sax 1986)
LD50 values to mammals in non-oral exposure, mg/kg	150 355 2260 56	unk-mam (Lewis & Sweet 1984) ipr-rat scu-rat ivn-mus (Sax 1986)
TDLo values to mammals in non-oral exposure, mg/kg	6700	skn-mus, 16W-I, tumorigenic (Sax 1986)
Health effects	No serious health hazards in normal industrial use. No systemic hazard incidental to industrial use unless harmful amounts are obtained by swallowing of substantial quantities. Large amounts of dust and fumes from heated material may cause pain and irritation of the eyes and nose, but they present no appreciable hazard, There is a possibility of skin irritation, but no danger of poisoning by skin absorption (Sax 1986). A 5% solution in sesame oil was mildly irritating in a few of 200 individuals upon prolonged contact. No evidence of sensitization. Solid irritates skin on prolonged contact. Dust may cause swelling of eyes and eye injury; irritation of nose and throat. Decreased activity, motor weakness, convulsive seizures (Sax 1986).	
Mutagenicity	Ames assay; Salmonella typhimurium; 0.5, 5, 50 or 500 μg/plate; 2,4,5-TCP was non-mutagenic with and without a metabolic activation system (Sax 1986). Plant cytogenetics; Vicia faba; spray; 7 cc (63 ppm), daily, 5 days; 1,27% and 1.38% mean abnormal pollen mother cells were observed in plants treated at 15 or 35 old, respectively. Abnormalities in pollen mother cells included stickiness and lagging of chromosomes during cell division and chromosome fragments (Sax 1986).	
Teratogenicity	Mus; orl; 0.0, 0.9 or 9.0 mg/kg; days 6–15 or gestation; there were no significant teratogenic effects at either dose level (Sax 1986).	
Effects on plants	Applied as herbicide to rice at 2, 3, or 5 kg/ha. Woedar (45% 2,4,5-TCP) gave 63.45, 65.62 or 69.92% starch, respectively, compared to 68.85% in controls. Crude protein was 8.81, 8.31 and 8.25% respectively, compared to 8.56 in controls. Ash was 1.48, 1.12 and 1.53% respectively, with 1.66% in controls. Sprayed on cotton plants at flowering increased height and number of fruiting nodes (Sax 1986).	
Effects on microorganisms	Compounds containing 5–10 wt % of a mixture of 2,4,5-TCP and either neomycin sulfate (in a wt ration of 97–67: 3–33, resp.) or polymyxin B sulfate (in a wt ratio of 80–3: 20–9, resp.) have potential antimicrobial activity (Sax 1986).	
EC50 values to algae, mg/l	1.22 0.89 0.96	96hr, Selenastrum capricornutum chlorophyll A 96hr, Skeletonema costatum chlorophyll A 96hr, Skeletonema costatum cell count (Sax 1986)

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LC50 values to crustaceans, mg/l	0.78	48hr, Daphnia magna (LeBlanc 1980)
	2.66 3.83	Daphnia magna 96hr, mysid shrimp (Sax 1986)
	3.6	7d, Daphnia magna (LeBlanc et al. 1988)
EC50 values to crustaceans, mg/l	2.7	48hr, Daphnia magna (Sax 1986)
	0.89	7d, Daphnia magna (LeBlanc et al. 1988)
LC50 values to fishes, mg/l	0.45	96hr, Lepomis macrochirus (Buccafusco et al. 1981)
	1.7	96hr, Cyprinodon variegatus (Heitmuller et al. 1981)
	1.7 1.3	24hr, Carassius auratus, 48hr, Leuciscus idus (Kobayashi 1979)
	1.66	96hr, Cyprinodon variegatus (Sax 1986)
	1 9	48hr, Salmo gairdneri 24hr, Carassius auratus (Sax 1986)
	2.4	48hr, Oryzias latipes (MITI 1992)
Other information about water organisms	EC50 (24hr) 0.68 mg/l, rpd, Tetrahymena pyriformis (Yoshio ka et al. 1985). 10 ppm, complete destruction of chlorophyll in the freshwater alga Chlorella pyrenoidosa. – 1.659 ppm, LC50 for chlorosis in duckweed (Sax 1986). Salmo gairdneri, 1 mg/l, 48hr, lowest concentration killing at least 50%. – Lymnaied snail, 10 mg/l, 24hr, 100% mortality (Sax 1986).	
Other information	2,4,5-TCP was an inhibitor of both p-nitroanisole demethylation and EPN detoxification in vitro. – 2,4,5-TCP had some inhibiting effect on fungal cell growth in tests carried out in submerged culture, and on an agar plate. It caused little cell damage. – The spreading of trichal blue algae (Phormidium) on culture medium in a petri dish was completely inhibited by 0.100 mg/spot 2,4,5-TCP. – Chlorophenol prevent the transfer of nonpersistent viruses by acting as repellents for the vector aphids. – The herbicide 2,4,5-TCP had an inhibitory effect at concentrations > 100 ppm on dairy cultures. – 2,4,5-TCP decreased the concentration of glycolysis metabolites and free adenine nucleotides in bovine lenses in vitro, indicating an impairment of energy supply. It had no effect on the activity of some enzymes required for carbohydrate breakdown. – The conductivity of bimolecular membranes artificially prepared from phospholipids of brain, bull heart and Micrococcus lysodeikticus biomass were measured in the presence of selected uncouplers of oxidative phosphorylation, including 2,4,5-TCP. The conductivities of brain and mitochondrial membranes increased similarly. 2,4,5-TCP had a greater influence on mitochondrial membranes. All chemicals tested also increased the conductivity of bacterial membranes. – 2,4,5-TCP in an effective -SH group inhibitor in enzymes of wood-rotting fungi. – 2,4,5-TCP at a concentration of 0.05 mM completely uncoupled or inhibited mitochondria at a mitochondrial concentration of 5 mg protein per mL. Albumin is effective in countering this inhibitory action. – 2,4,5-TCP was pyrolysed, and the pyrolysates (0.00025 mg/egg) were injected into the air cell of fresh fertile eggs before incubation. Solvents used were ethanol, acetone and chloroform. At 21 days, there was 50% mortality. The mortality of non-injected and solvent injected controls was 10–15%. – The inhibition of oxidative phosphorylation by 50% was shown at a concentration of 3E-6 M in rat liver mitochondria. Measurement was via oxygen consumption using polarographic techniques (Sax 1986).	

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1954 • 2,4,6-Trichlorophenol

88-06-2

Synonyms	Dowicide 25 Phenachlor 2,4,6-T Trichlorophenol 2,4,6-TCP 1,3,5-Trichlorophenol	
Sumformula of the chemical	C6H3Cl3O	
Purity, %	97	
Known impurities	Sometimes:1,3,6,8-tetrachlorodibenzo-p-dioxin 2,3,7-trichlorodibenzo-p-dioxin-tri-, tetra-, and pentachlorodimethoxydibenzofuranstetra-, hexa-, penta-, and heptachlorodibenzofurans	
Use	Bactericide; fungicide; germicide; manufacturing of antiseptics and wood and glue preservatives.	
State and appearance	Needles or solid. Yellow, pinkish-orange.	
Odour	Strong phenolic odour.	
Molecular weight	197.44	
Specific gravity (water=1)	1.675 1.49	
Vapour pressure, mmHg	1	at 76.5 °C
Water solubility, mg/l	800 434 800	25 °C 20 °C (Blackman et al. 1955) 25 °C (Mabey et al. 1982)
Melting point, °C	69.5	(Suntio et al. 1988)
Boiling point, °C	244.5	
Flashing point, °C	61	
pKa	6.42 7.42 5.99	 (Doedens 1967) (Ugland et al. 1981)
Log octanol/water coefficient, log Pow	3.62–4.05 3.69 3.38 3.72 3.79 3.62 3.69 4.05	(Sax 1986) (Anon. 1986) observed (Chin et al. 1986) (Xie 1984) (Hansch & Leo 1979) (Hansch & Leo 1979) (Hansch & Leo 1979) (Hansch & Leo 1979)
Log soil sorption coefficient, log Kom	3.02 2.99	observed (Sabljic 1987) calculated (Sabljic 1987)
Henry's law constant, Pa x m³/mol	0.2424	calc. (Suntio et al. 1988)
Mobility	7.08% (air), 73.36% (water), 19.56% (sediment). Moderately acidic and will exist as an anion (Sax 1986).	

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Aerobic degradation in soil	AEROBIC DEGRADATION IN SOIL Maximum adsorption wavelength: 289 nm NON-STERILE SOIL Minimum time for > 70% decrease: 1.50–2.00 d % decomposition at the termination of the experiment: 3d, 95% STERILE SOIL % decomposition at the termination of the experiment: 80d, 27% (Baker et al. 1980)
Anaerobic degradation in soil	ANAEROBIC DEGRADATION IN SOIL Maximum adsorption wavelength: 289 nm NON-STERILE SOIL % decomposition at the termination of the experiment: 80d, 28% STERILE SOIL % decomposition at the termination of the experiment: 80d, 25% (Baker et al. 1980)
Total degradation in soil	Decomposition in soil suspensions: 5 days for complete disappearance (Verschueren 1983).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
Other information about degradation	Degradation by Pseudomonas (200 mg/l, 30 °C): parent: 100% ring disruption in 120 hours mutant: 100% ring disruption in 50 hours (Verschueren 1983).

In the presence of an electron acceptor, can be photoxidized to 2,6-dichlorobenzoquinone and 2,6-dichlorohydroquinone, although the relevance of this to environmental systems is uncertain. Sorption to organic detritus but not sedimentary clays, may be important. Oxidation, hydrolysis, and volatilization unlikely to be important. Biodegradation by sewage sludge and soil samples have been demonstrated, but no studies done with aquatic systems. In repeat batch experiments, the number of days to obtain 70% degradation of 1 ppm in mineral water was 9 to 18 days; 26 to 65 days in seawater (Sax 1986).

Degradation of 2,4,6-trichlorophenol:

ENVIRONMENT	*INIT.CONC. mg/l*	*REDOX-COND.*	*TEMP. °C*	*DEGRADATION %/day*	*REF.*
water	5	aerobic	25	100/7	a
water	10	aerobic	25	100/7	a
water (PCP ad.)	–	aerobic	–	100/1	b
groundwater	1	aerobic	–	95/13	c
groundwater	1	aerobic	–	60/3	c
groundwater	1	aerobic	–	45/9	c
groundwater	1	aerobic	–	77/13	c
sludge	20	anaerobic	37	100/7	d
sludge	20	anaerobic	37	100/28	d
sludge	700	anaerobic	–	appr. 45/75	e
sludge	4000	aerobic	37	70/125	e
soil suspension	10–100	aerobic	30	100/5	f
soil suspension	10–100	aerobic	30	100/13	f
soil	1	aerobic	23	95/3	g
sterile soil	1	aerobic	23	27/80	g
soil	1	anaerobic	23	28/80	g
sterile soil	1	anaerobic	23	8/80	g

a) Tabak et al. 1981
b) Steiert & Crawford 1985
c) Suflita & Miller 1985
d) Mikesell & Boyd 1985
e) Kincannon & Lin 1985
f) Alexander & Aleem 1961
g) Baker & Mayfield 1980
(Anon. 1987b).

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Metabolism in mammals	Male rats were fed 3 subsequent daily doses (via stomach tube) of 1 mg/kg diet. During the elimination phase of 5 days the radioactivity in the feces and in the urine was measured. Results: elimination via urine was 32.3% of applied amount (30.6% during the elimination phase) and elimination via feces was 22.2% of applied amount (9.4% during the elimination phase). After the elimination phase the rats were sacrificed and tissue samples were taken to determine the amount stored as a percentage of applied amount per gram. No detectable level was found in liver, lung, or fatty tissue (Sax 1986).
Bioconcentration factor, fishes	20 Carassius auratus (Verschueren 1983)
LD50 values to mammals in oral exposure, mg/kg	820 orl-rat 454 orl-man (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	700 skn-mam (Lewis & Sweet 1984) 276 ipr-rat (Sax 1986)
TDLo values to mammals in oral exposure, mg/kg	185000 orl-rat, 2Y-C, tumorigenic 441000 orl-mus, 2Y-C, tumorigenic (Sax 1986)
Effects on the physiology of mammals	2,4,6-TCP was found to inhibit proline an d glycine transport by binding at specific sites on proteins with the free energy of interaction stabilizing 'unproductive' conformations. – 2,4,6-TCP was designated as an uncoupler of oxidative phosphorylation in mitochondia. It was applied to neurons in an isolated ganglion of marine mollusc (Navanox inermis) and caused a rapid, reversible, dosedependent increase in the membrane potential and conductance, due to the relative increase in conductance of potassium (relative to chloride). It also produced a reversible dosedependent decrease in the mermeability or alkali-cations relative to potassium. – 2,4,6-TCP inhibited B-D-galactoside transport in Escherichia coli in proportion to its concentration starting at 0.010 mg/ml for 10 minutes. – 2,4,6-TCP was one of a number of phenols which caused an increase in biliary excretion of harmol glucuronide, presumably by inhibition of sulfation of harmol (in rats). – 2,4,6-TCP was found to inhibit chloride transport in RBC's (mammalian) by 50% at a concentration of 1.32E-5 M. – The inhibition of oxidative phosphorylation by 50 % was shown at a concentration of 18E-6 M in rat liver mitochondria. – 2,4,6-TCB showed an inhibitory effect on C-oxygenation, while not having such a pronounced effect on N-oxygenation in rat liver microsomes that were being tested for selective inhibition of the terminal oxygenation enzyme P-450. The qualitative shift in detoxification of DMA (N,N-dimethylaniline) from C to N-oxygenation was considered as a possible synergist for the carcinogenic action of aromatic amines (Sax 1986).
Health effects	Trichlorophenols can produce redness and edema on skin contact and with prolonged exposure can produce mild to moderate chemical burns to human skin. In the eye they induce conjuctival irritation and sometimes corneal injury and iritis. The dusts are irritating to the nose and pharynx. Systemic effects are not described but presumably resemble those of phenol poisoning. – 2,4,6-TCP has a permeability coefficient of 9.9E4 cm/min for human epidermis. – 2,4,6-TCB showed 77% stripping of human spermatozoa at a concentration of 11.0 pmol/cell. Stripping consisted of removal of the peripheral cytoplasm leaving the nucleus and tail fibers to form the 'sperm core' (Sax 1986). Skin and eye irritation data: skn, rbt, 500 mg, 24hr, moderate; eye, rbt, 0.250 mg, 24hr, severe (Sax 1986).
Carcinogenicity	NCI carcinogenesis bioassay completed: results positive: mus, rat (Lewis & Sweet 1984).
Mutagenicity	Mutagen data: mmo, sat, 0.400 ml/plate (Sax 1986).
Effects on arthropods	Tanytarsus dissimilis, LC50, 2 d, > 13.5 mg/l (Holcombe et al. 1987).

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Effects on wastewater treatment	In flask culture inoculated with sewage bact eria, 7–10 days were required to remove 95% of the initial 300 ppm 2,4,6-TCP; 3 hours for 70% removal of 100 ppm. With acclimated sludge, complete ring degradation in 5 days (Sax 1986).	
EC50 values to algae, mg/l	5.6	96hr, grw, Scenedesmus subspicatus (Geyer et al. 1985)
	10	96hr, grw, Chlorella vulgaris
	3.5	96hr, grw, Selenastrum capricornutum (Shigeoka et al. 1988)
LC50 values to crustaceans, mg/l	6	48hr, Daphnia magna (LeBlanc 1980)
	0.69	48hr, Daphnia magna (Kukkonen & Oikari 1987)
EC50 values to crustaceans, mg/l	3.34	2d, mbt, Daphnia magna (Holcombe et al. 1987)
	15	24hr, Daphnia magna
	6	48hr, D.magna (Sax 1986)
LC50 values to fishes, mg/l	2.6	96hr, pH 7.3–8.1, Salmo gairdneri
	0.45	96hr, pH 6.4, Salmo gairdneri (Voss et al. 1981)
	0.1–1.0	96hr, Pimephales promelas (Könemann 1979)
	10	24hr, Carassius auratus (Kobayashi 1979)
	0.32	96hr, Lepomis macrochirus (Buccafusco et al. 1981)
	7.7	48hr, Pimephales promelas
	5.8–6.4	192hr, Pimephales promelas (Phipps et al. 1981)
	0.41	4d, Lepomis macrochirus
	2.74	4d, Pimephales promelas
	0.73	4d, Salmo gairdneri (Holcombe et al. 1987)
	0.6	96hr, Pimephales promelas
	9.04	96hr, P.promelas, juvenile (Sax 1986)
	4.55	96hr, Pimephales promelas (Geiger et al. 1988)
Effects on the physiology of water organisms	Salmo gairdneri, 4 d, 0.2 mg/l, change in enzyme activity (Castren & Oikari 1987).	
Other information about water organisms	Aplexa hypnorum, LC50, 4 d, 5.5 mg/l (Holcombe et al. 1987). LC50 for chlorosis in duckweek (Lemna mi nor) was 5.9 mg/l. – Photosynthetic supression in Chlorella pyre noidosa (measured by rates of oxygen evolution) was 53.2%, as compared to the control at 50 mg/l. The concentration at which no substantial toxicity occurred was 1.0 mg/l. The tests were conducted under steady-state conditions, algal density of 1 g/l (dry weight), 25 °C, aerated, with constant light for 72hr (Sax 1986). Lymnaied sp., effect level, 24hr, 5.0 mg/l (Sax 1986).	
Other effects on aquatic ecosystems	Taste threshold; 0.002 mg/l in water; 48hr threshold limit for taste impairment in rainbow trout is 0.052 mg/l (Sax 1986).	

1955 • 3,4,5-Trichlorophenol 609-19-8

Log octanol/water coefficient, log Pow	3.69–4.41	(Sabljic 1987)
Log soil sorption coefficient, log Kom	3.56	observed (Sabljic 1987)
	2.99	calculated (Sabljic 1987)

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Aerobic degradation in soil	AEROBIC DEGRADATION IN SOIL Maximum adsorption wavelength: 295 nm NON-STERILE SOIL % decomposition at the termination of the experiment: 160d, 17% STERILE SOIL % decomposition at the termination of the experiment: 160d, 0% (Baker et al. 1980)
Anaerobic degradation in soil	ANAEROBIC DEGRADATION IN SOIL Maximum adsorption wavelength: 295 nm NON-STERILE SOIL % decomposition at the termination of the experiment: 80d, -2% STERILE SOIL % decomposition at the termination of the experiment: 80d, 4% (Baker et al. 1980)
Other information about degradation	Degradation of 3,4,5-trichlorophenol:

ENVIRONMENT	*INIT.CONC. mg/l*	*REDOX-COND.*	*TEMP. °C*	*DEGRADATION %/day*	*REF.*
water (PCP-ad.)	–	aerobic	–	0/1	a
soil	1	aerobic	23	17/160	b
sterile soil	1	aerobic	23	0/160	b
soil	1	anaerobic	23	0/80	b
sterile soil	1	anaerobic	23	4/80	b

a) Steiert & Crawford 1985 b) Baker & Mayfield 1980
(Anon. 1987b).

LC50 values to fishes, mg/l	1.1	24hr, Poecilia reticulata (Könemann 1979)

1956 • 2,3,6-Trichlorophenyl acetic acid 85-34-7

LC50 values to crustaceans, mg/l	4.5 6.6	48hr, Daphnia pulex 48hr, Simocephalus serrulatus (Sanders & Cope 1966)
LC50 values to fishes, mg/l	15	48hr, Lepomis macrochirus (Hughes & Davis 1962)

1957 • 1,2,3-Trichloropropane 96-18-4

Use	Solvent.	
Water solubility, mg/l	960	(MITI 1992)
Boiling point, °C	156.9	(MITI 1992)
Log octanol/water coefficient, log Pow	2.27	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	5.4–12 5.3–13	8w, Cyprinus carpio, conc 0.2 mg/l 8w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)

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Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	320	orl-rat
LC50 values to fishes, mg/l	42	7d, Poecilia reticulata (Könemann 1979)
	109	48hr, Oryzias latipes (MITI 1992)

1958 • Trichlorotrifluoroethane 76-13-1

Synonyms	Freon 113 Ucon-113 solvent	
Use	Solvent.	
Odour	Quality: sweet Hedonic tone: pleasant to unpleasant Threshold odour concentration absolute: 45.0 ppm 50% recognition: 68.0 ppm 100% recognition: 135.0 ppm Odour index 100% recognition: 54 (Hellman & Small 1974).	
Water solubility, mg/l	100	20 °C
	120	(MITI 1992)
Boiling point, °C	46	
Log octanol/water coefficient, log Pow	2.97	(MITI 1992)
Volatilization	Relative volatility (nBuAc=1) = 40.7	
Total degradation in water	Biodegradation: 0–5% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	11–33	6w, Cyprinus carpio, conc 0.198 mg/l
	14–86	6w, Cyprinus carpio, conc 0.0198 mg/l (MITI 1992)
LD50 values to mammals in oral exposure, mg/kg	45	orl-rat
LC50 values to fishes, mg/l	40.8	48hr, Oryzias latipes (MITI 1992)

1959 • Trichlorphon 52-68-6

Synonyms	Chlorophos O,O-Dimethyl-2,2,2-trichloro-1-hydroxyethylphosphonate Trichlorfon O,O-Dimethyl-(2,2,2-trichloro-1-hydroxyethyl)phosphonate
Sumformula of the chemical	C4H8Cl3O4P
Products containing the chemical	Tugon-muurahaissirote * trichlorphon 10g/kg (PESREG)
Use	Active ingredient in insecticides.

Instructions for handling	Stable (full biological effect, < 40 °C) for 24 months. (Tugon-muurahaissirote *) (PESREG)
State and appearance	Solid, crystalline, white. (PESREG)
Odour	Slight odour. (PESREG)
Particle size, mm	> 0.3 maximum refuse to the sieve: 95% > 1.0 maximum refuse to the sieve: 5% (Tugon-muurahaissirote *) (PESREG)
Molecular weight	257.44
Specific gravity (water=1)	1.73 (PESREG)
Vapour pressure, mmHg	0.0000078 20 °C 0.000028 30 °C 0.000111 40 °C (PESREG)
Water solubility, mg/l	154000 25 °C 123000 15 °C (PESREG)
Fat solubility, g/100g	1.493 37 °C (PESREG)
Melting point, °C	81–84
Boiling point, °C	100 0.1 mmHg 109 0.2 mmHg 120 0.4 mmHg (PESREG)
Log octanol/water coefficient, log Pow	0.43 (PESREG)
Other physicochemical properties	Soluble easily in polar organic solvents. *Solubility (g/100g at 20 °C)* dichloromethane > 20 n-hexane 0.01–0.1 2-propanol > 20 toluene 13 (PESREG).
Photochemical degradation in soil	In two photo lysis (irradiated with simulated sunlight) studies of silt loam soil half-lives of trichlorphon were 9–11.8 days. The half-lives of control samples (in the dark) were 10–12.8 days. The major degradation products were identified as 2,2-dichlorvinyl dimethyl phsphate and 2,2-dichlorovinyl, O-methyl phosphate. (PESREG)
Photochemical degradation in water	The photolysis (irridiated with simulated sunlight) half-life of trichlorphon in an aqueous buffer solution (pH 5) was 110 days. The half-life of control sample (in the dark) was 115 days Degradation products were identified as 2,2-dichlorovinyl dimethyl phosphate, 2,2-dichlorovinyl O-methyl phosphate and dichloroacetaldehyde. (PESREG)
Hydrolysis in water	The hydrolysis half-lives of trichlorfon in buffered solutions

half-life

	20 °C	22 °C	30 °C	40 °C	70 °C	80 °C	90 °C
pH 4		510d*			24hr	8.7hr	3hr
pH 7		46hr*	14hr	3.2hr			
pH 9	< 30min	< 30min*					

* calculated

Hydrolysis products were demethyl-trichlorfon, dichlorvos, demethyl-dichlorvos, chloral, methyl phosphite and phosphoric acid in acid and basic medium. (PESREG)

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Degradation and transformation products	2,2-dichlorovinyl dimethyl phosphate 2,2-dichlorovinyl, O-methyl phosphate dichloroacetaldehyde demethyl-trichlorfon dichlorvos demethyl-dichlorvos chloral methyl phosphite phosphoric acid	
LD50 values to mammals in oral exposure, mg/kg	150	orl-rat (Lewis & Sweet 1984)
	150–700	orl-rat (PESREG)
	212–258	orl-rat (PESREG)
	734	orl-mus (PESREG)
	> 300	orl-dog male (PESREG)
	540–630	orl-rat (PESREG)
	680–730	orl-mus (PESREG)
LD50 values to mammals in non-oral exposure, mg/kg	2000	skn-rat (Lewis & Sweet 1984)
	> 5000	7d, idr-rat (PESREG)
	> 5000	14d, idr-rat (PESREG)
	> 5000	14d, idr-mus (PESREG)
	410–485	ipr-rat (PESREG)
	344–354	ipr-mus (PESREG)
LC50 values to mammals in inhalation exposure, mg/m³	1.3	ihl-rat (Lewis & Sweet 1984)
	> 419	1hr, ihl-rat (PESREG)
	> 533	4hr, ihl-rat (PESREG)
LD50 values to birds in oral exposure, mg/kg	40	orl-bwd (Lewis & Sweet 1984)
	37.0–75.0	orl-Agelaius phoeniceus
	43	orl-Sturnus vulgaris (Schafer et al. 1983)
LDLo values to birds in oral exposure, mg/kg	80	orl-ckn (Lewis & Sweet 1984)
	0.05	10 d, Dunaliella euchlora (Ukeles 1962)
LC50 values to crustaceans, mg/l	0.001	48hr, Crassostrea virginica (Davis & Hidu 1969)
	0.00032	48hr, Simocephalus serrulatis
	0.00018	48hr, Daphnia pulex (Sanders 1972)
	31	96hr, Saccobranchus fossilis (Verma et al. 1982)
	0.00012	act, Daphnia pulex (Frear & Boyd 1967)
	0.0004	48hr, Daphnia magna (Gorbach & Knauf 1971)
	0.065	act, Daphnia pulex (Nishiuchi & Hashimoto 1967)
	0.13	24hr, Daphnia magna
	0.08	48hr, Daphnia magna (Ardo 1974)
	0.00012	act, Daphnia magna (Kenaga 1979)
	0.2	4d, Procambarus clarkii (Andreu-Moliner et al. 1986)
EC50 values to crustaceans, mg/l	0.00007	48hr, Daphnia pulex (Shapiro 1967)

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LC50 values to fishes, mg/l	1.4 0.26 51	act, Salmo gairdneri act, Lepomis macrochirus act, Pimephales promelas (Kenaga 1979)
	8.8	24hr, Cyprinus carpio (Hashimoto et al. 1982)
	3.2	96hr, Salmo clarci (Woodward & Mauck 1980)
	3.8	96hr, Lepomis macrochirus (Mount & Stephan 1967)
	4.85	96hr, Salmo gairdneri (Marking & Mauck 1975)
	6.2	48hr, Cyprinus carpio (Nishiuchi & Hashimoto 1967)
Other information about water organisms	EC (10d) 0.05 mg/l, rpd, Dunaliella euchlora; Chlorella sp.; Monochrystis lutheri (Ukeles 1962). LC50 (96hr) 0.069 mg/l, Pteronarcys californica LC50 (30d) 0.0098 mg/l, Pteronarcys californica (Jensen & Gaufin 1964).	

1960 • Triclopyr 55335-06-3

Log soil sorption coefficient, log Kom	1.43	(Sabljic 1987)
EC50 values to crustaceans, mg/l	1.2	4d, mbt, Daphnia pulex (Servizi et al. 1987)
LC50 values to fishes, mg/l	13.3 5.3 7.9 7.5 9.9 9.6 7.8 7.5 9.7 9.7 8.4 7.5	1d, Oncorhynchus gorbuscha 4d, Oncorhynchus gorbuscha 1d, Oncorhynchus keta 4d, Oncorhynchus keta 1d, Oncorhynchus kisutch 4d, Oncorhynchus kisutch 1d, Oncorhynchus nerka 4d, Oncorhynchus nerka 1d, Oncorhynchus tshawytscha 4d, Oncorhynchus tshawytscha 1d, Salmo gairdneri 4d, Salmo gairdneri (Wan et al. 1987)
	2.2 1.2 1.4 2.2	4d, Oncorhynchus kisutch 4d, Oncorhynchus nerka 4d, Oncorhynchus nerka 4d, Salmo gairdneri (Servizi et al. 1987)

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1961 • p-Tricresyl phosphate 1330-78-5

Sumformula of the chemical	C21H2104P
Total degradation in water	Biodegradation: 100% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).

1962 • Tricyclohexyltin hydroxide 13121-70-5

Synonyms	Cyhexatin	
Use	Acaricide.	
Molecular weight	385.21	
LD50 values to mammals in oral exposure, mg/kg	180	orl-rat (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	1880	skn-rat (Lewis & Sweet 1984)
Other information about mammals	LDfr = 37.5 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).	
LD50 values to birds in oral exposure, mg/kg	654	orl-ckn (Lewis & Sweet 1984)
LC50 values to crustaceans, mg/l	0.03	act, Daphnia magna (Kenaga 1979)
LC50 values to fishes, mg/l	0.001 0.008 0.06 0.55	act, Salmo gairdneri act, Lepomis macrochirus (Kenaga 1979) 24hr, Large-mouth bass 24hr, Carassius auratus (Pesticide Manual 1983)

1963 • Tridecyl alcohol 112-70-9

Synonyms	1-Tridecanol	
Sumformula of the chemical	C13H28O	
EINECS-number	2039988	
Melting point, °C	30.5	(MITI 1992)
Boiling point, °C	155–156	15 mmHg (MITI 1992)
Total degradation in water	Biodegradation: 76.8–100% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	

1964 • Trietazine 1912-26-1

Use	Herbicide.	
Log soil sorption coefficient, log Kom	2.78	(Sabljic 1987)
LC50 values to crustaceans, mg/l	> 40	act, Daphnia pulex (Nishiuchi & Hashimoto 1967)
LC50 values to fishes, mg/l	0.85	48hr, Cyprinus carpio (Nishiuchi & Hashimoto 1967)

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1965 • Triethanolamine 102-71-6

Melting point, °C	21.2	(MITI 1992)
Boiling point, °C	360.8	(MITI 1992)
Chemical oxygen demand, g 02/g	1.53	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.08	5 days (Bridie et al. 1979)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.4 < 3.9	6w, Cyprinus carpio, conc 2.5 mg/l 6w, Cyprinus carpio, conc 0.25 mg/l (MITI 1992)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): > 10000 mg/l (Bringmann & Kühn 1980a).	
LOEC values to algae, mg/l	1.8 47	rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a) rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to fishes, mg/l	75000 > 5000 > 1000	24hr, Carassius auratus (Anon. 1975) 24hr, Carassius auratus (Bridie et al. 1979) 48hr, Oryzias latipes (MITI 1992)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 1.8 mg/l protozoa (Entosiphon sulcatum): 56 mg/l (Bringmann & Kühn 1980a).	

1966 • Triethyl phosphate 78-40-0

Synonyms	Triethylphosphate	
Boiling point, °C	216	(MITI 1992)
Log octanol/water coefficient, log Pow	0.77	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	0.5–0.8 < 1.3	6w, Cyprinus carpio, conc 1 mg/l 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to crustaceans, mg/l	950	96hr, 10 °C, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	2100 > 500	96hr, 10 °C, Alburnus alburnus (Linden et al. 1979) 48hr, Oryzias latipes (MITI 1992)

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1967 • Triethylamine

121-44-8

Synonyms	(Diethylamino)ethane N,N-Diethylethanamine
Sumformula of the chemical	C6H15N
Use	Catalytic solvent in chemical synthesis; accelerator activators for rubber; wetting, penetrating, and waterproofing agents of quaternary ammonium types; curing and hardening of polymers (e.g., corebinding resins); corrosion inhibitor; propellant.
State and appearance	Colourless liquid.
Odour	Strong ammoniacal odour. Characteristic: quality: fishy, amine. Hedonic tone: unpleasant to pleasant. T.O.C.: abs. perc. lim.: < 0.09 ppm; 50% recognition: 0.28 ppm; 100% recognition: 0.28 ppm; O.I. 100% recognition: 253.6 (Verschueren 1986). Quality: fishy, amine Hedonic tone: unpleasant to pleasant Threshold odour concentration absolute: < 0.09 ppm 50% recognition: 0.28 ppm 100% recognition: 0.28 ppm Odour index 100% recognition: 253 571 (Hellman & Small 1974).
Molecular weight	101.22
Specific gravity (water=1)	0.723 25/4 °C
Vapour density (air=1)	3.48
Conversion factor, 1 ppm in air=	4.29 mg/m³
Conversion factor, 1 mg/m³ in air=	0.24 ppm
Vapour pressure, mmHg	50 20 °C
Water solubility, mg/l	15000 20 °C 19700 65 °C 82000 (MITI 1992)
Melting point, °C	-144.75 (MITI 1992)
Boiling point, °C	89–90 89.4 (MITI 1992)
Flashing point, °C	-6.67
pKa	10.76 (Sangster 1989)
Log octanol/water coefficient, log Pow	1.44 1.45 (Sangster 1989) 0.87 (MITI 1992)
Volatilization	Relative volatility (nBuAc=1) = 5.60
Other physicochemical properties	Soluble in water and alcohol. Hazard: Flammable, dangerous fire risk, explosive limits in air 1.2–8.0%. Toxic by ingestion and inhalation, strong irritant to tissue.

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Total degradation in water	Biodegradation: 25–34% by BOD period: 28d substance: 30 mg/l sludge 100 mg/l (MITI 1992).
Other information about degradation	Impact on biodegradation processes: inhibition of degradation of glucose by Pseudomonas fluorescens at: 600 mg/l; inhibition of degradation of glucose by Escherichia coli at: < 1000 mg/l (Verschueren 1983). NH3 oxidation by Nitrosomonas sp.: at 100 mg/l: 35% inhibition; at 127 mg/l: appr. 50% inhibition (Verschueren 1983). Biodegradation; degradation by Aerobacter; 200 mg/l at 30 °C: parent: 100% in 28hr; mutant: 100% 11hr (Verschueren 1986).
Bioconcentration factor, fishes	< 0.5 6w, Cyprinus carpio, conc 0.5 mg/l < 4.9 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
LD50 values to mammals in oral exposure, mg/kg	460 orl-rat 546 orl-mus (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	570 skn-rbt (Sweet 1987)
LC50 values to mammals in inhalation exposure, mg/m³	6000 ihl-mam (Sweet 1987)
LCLo values to mammals in inhalation exposure, ppm	1000 ihl-gpg, 4hr ihl-rat, 4hr 1000 ihl-gpg, 4hr ihl-rat, 4hr (Sweet 1987)
TDLo values to mammals in oral exposure, mg/kg	6.9 orl-rbt, 1-3d preg, eff. on fertility (Sweet 1987)
Health effects	Skin and eye irritation data: skin, rbt, 10 mg, 24hr, open, mild; skin, rbt, 365 mg, open, mild; eye, rbt, 250 mg, open. severe; eye, rbt, 50 ppm, 30 D-I, severe (Sweet 1987).
Mutagenicity	Mutation data: cytogenic analysis; rat, ihl, 1 mg/m³ (Sweet 1987).
LD50 values to birds in oral exposure, mg/kg	> 100 orl-Agelaius phoeniceus (Schafer et al. 1983)
Effects on microorganisms	Escherichia coli: no effect; 1 g/l (Verschueren 1986).
LC50 values to fishes, mg/l	50.7 48hr, Oryzias latipes (MITI 1992)
Other information about water organisms	Fish: Semolitus atromaculatus (Creek chub), LD100, 80 mg/l, 24hr, in Detroit river water (Verschueren 1986).

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1968 • Triethyleneglycol 112-27-6

Synonyms	3,6-Dioxaoctane-1,8-diol
Sumformula of the chemical	C6H14O4
Use	Solvent and plasticizer in vinyl, polyester, and polyurethane resins; dehydration of natural gas; humectant in printing inks; extraction solvent.

State and appearance	Colourless, hygroscopic, practically odourless liquid.
Specific gravity (water=1)	1.1254 20/20 °C
Water solubility, mg/l	> 100000 (MITI 1992)
Melting point, °C	9.4 (MITI 1992)
Boiling point, °C	287.4 278.31 (MITI 1992)
Flashing point, °C	176.6
Other physicochemical properties	Autoign temperature 371 °C, soluble in water, immiscible with benzene, toluene and gasoline. Combustible.
Chemical oxygen demand, g 02/g	1.57 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.03 5 days (Bridie et al. 1979)
Total degradation in water	Biodegradation: 25–92% by BOD (on the upward trend) period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 320 mg/l (Bringmann & Kühn 1980a).
LOEC values to algae, mg/l	3600 rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to crustaceans, mg/l	35000 48hr, Daphnia magna (LeBlanc & Surprenent 1983)
LC50 values to fishes, mg/l	> 10000 96hr, Lepomis macrochirus Menidia audens (Dawson et al. 1977) > 5000 24hr, Carassius auratus (Bridie et al. 1979)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): > 10000 mg/l protozoa (Entosiphon sulcatum): > 10000 mg/l (Bringmann & Kühn 1980a).

1969 • Triethyleneglycol monoethylether 112-50-5

Synonyms	1-Methoxy-3,6-dioxaoctan-8-ol
Sumformula of the chemical	C8H1804
Chemical oxygen demand, g 02/g	1.84 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.05 5 days (Bridie et al. 1979)
LC50 values to fishes, mg/l	> 5000 Carassius auratus (Bridie et al. 1979)

1970 • Triethyleneglycoldi(2-ethylbutyrate) 141-17-3

Synonyms	Hexanedioic acid, bis(2-(2-butoxyethoxy)ethyl) ester
Sumformula of the chemical	C22H4208

EINECS-number	2054655
Melting point, °C	< -10 (MITI 1992)
Boiling point, °C	> 300 (MITI 1992)
Total degradation in water	Biodegradation: 79–84% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

1971 • Triethyllead chloride 1067-14-7

LC50 values to fishes, mg/l	1.7 as Pb, 96hr, Platichthys flesus 9 as Pb, 96hr, Salmo gairdneri (Maddock & Taylor 1977)
Effects on the physiology of water organisms	0.006 mM, EC50, phy, 0.13 d, Poteriochromonas malhamensis (Roderer 1986).
Other information about water organisms	LC50 (96hr) 1.1 mg Pb/l, mussel (Maddock & Taylor 1977). 100% mortality: 0.005 M, 7 d, Chara vulgaris (Heumann 1987); 4.14 mg/l, 3 d, Poteriochromonas malhamensis (Roderer 1987).

1972 • Triethyltin bromide 2767-54-6

LC50 values to algae, mg/l	0.1 pht, Selenastrum quadricauda (Wong et al. 1982)

1973 • 3-Trifluoromethyl-4-nitrophenol 88-30-2

Synonyms	α,α,α-Trifluoro-4-nitro-m-cresol 4-Nitro-3-(trifluoromethyl)phenol
Use	To exterminate lampreys.
State and appearance	Crystals.
Molecular weight	207.12
Melting point, °C	74–76
Bioconcentration factor, other organisms	1.1–95.5 animals (Verschueren 1983)
LD50 values to mammals in oral exposure, mg/kg	500 orl-mam (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	25 ipr-mus (Lewis & Sweet 1984)
LC50 values to fishes, mg/l	5.95 96hr, Salvelinus alpinus 6.1 96hr, Salmo gairdneri (Dawson et al. 1977) 1.52 96hr, Salmo trutta m.lacustris, eggs 0.57 96hr, Oncorhynchus kisutch, eggs (Olson & Marking 1975)
Other information about water organisms	Protozoa, 1.0 mg/l, 28 d, change in ability to colonize an uninhibited substrate under toxicant stress (Cairns et al. 1986).

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1974 • 3-Trifluoromethyl-chlorobenzene

98-15-7

Sumformula of the chemical	C7H4ClF3
EINECS-number	2026429
Water solubility, mg/l	33 (MITI 1992)
Melting point, °C	-51.9 (MITI 1992)
Boiling point, °C	138.1 (MITI 1992)
Log octanol/water coefficient, log Pow	2.14 (MITI 1992)
Total degradation in water	Biodegradation (Closed Bottle Test): 0% by BOD period: 28d substance: 2.6 mg/l substance: 13.0 mg/l (MITI 1992).
Bioconcentration factor, fishes	90–214 8w, Cyprinus carpio, conc 0.1 m, g/l 191–260 8w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non–accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	17 48hr, Oryzias latipes (MITI 1992)

1975 • 3-(3-Trifluoromethylphenyl)-1,1-dimethylurea

2164-17-2

Sumformula of the chemical	C10H11F3N2O
Log soil sorption coefficient, log Kom	2.24 (Sabljic 1987)

1976 • Trifluralin

1582-09-8

Synonyms	Treflan 2,6-Dinitro-N,N-dipropyl-4-trifluoro-methylaniline α,α,α-Trifluoro-2,6-dinitro-N,N-dipropyl-4-toluidine
Sumformula of the chemical	C13H16F3N3O4
Products containing the chemical	Trifluralin 48 EC * 510 g trifluralin/l Super-Treflan * 480 g trifluralin/l Trinulan 12 * 240 g trifluralin/l + 240 g linuron/l
Purity, %	95 in technical product
Known impurities	Dichloronitro(trifluoromethyl)benzene isomer (0.8% w/w); N,N-Dipropyl-2,4-dinitro-6-(trifluoromethyl)benzenamine (0.35%); N,N-Dipropyl-dinitro(trifluoromethyl)benzenamine isomer (0.15%); N,N-Dipropyl-nitro(trifluoromethyl)benzenamine isomer (0.15%); 4-Chloro-3-nitro-1-(trifluoromethyl)benzene (0.14%)
Use	Active ingredient in herbicides.
State and appearance	Yellow orange solid.
Molecular weight	335.32

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Vapour pressure, mmHg	0.000199 29.5 °C
Water solubility, mg/l	4 27 °C
Melting point, °C	48.5–49.0
Boiling point, °C	139–140
Log octanol/water coefficient, log Pow	5.07 5.34 (Mackay 1982)
Log soil sorption coefficient, log Kom	4.14 (Sabljic 1987)
Half-life in soil, days	21 in irrigated soils in Texas 35 in Tennessee (Verschueren 1983) 132 (Li et al. 1990)
Total degradation in soil	Mean overwinter loss 38.1% in two sandy loam soils in Nova Scotia following application in November (Verschueren 1983).
Bioconcentration factor, fishes	1060–6000 (Verschueren 1983)
LD50 values to mammals in oral exposure, mg/kg	5000 orl-mus 3700 orl-mam (Lewis & Sweet 1984)
Carcinogenicity	NCI carcinogenesis bioassay completed: results positive;mus / response negative; rat (Lewis & Sweet 1984).
Effects on plants	0.56 kg trifluralin / ha a.i. reduced the fresh weight of weeds at harvest (Roberts & Bond 1975). Trifluralin was applied to vetch (Vicia sativa) and soybean (Glycine max) at 1 mg/kg dry soil immediately prior to potting. At that concentration trifluralin severely inhibited lateral root growth (O'Donovan & Prendeville 1977).
EC50 values to algae, mg/l	2.5 10 d, Chlorococcum sp. Phaeodactylum tricornutum (Walsh 1972)
LC50 values to crustaceans, mg/l	0.24 48hr, Daphnia pulex (Sanders & Cope 1966) 0.2 48hr, Asellus brevicaudus 0.56 48hr, srv, act, Daphnia magna 0.2 48hr, srv, act, Asellus brevicaudus (Sanders 1970) 0.56 D. magna (Kenaga 1979) 40 srv, act, D.pulex (Hashimoto & Nishiuchi 1981) 12 96hr, srv, act, Procambarus clarcii (Naqvi & Leung 1983) 0.06 srv, act, Cladocera 0.08 Calanoida 0.05 Cyclopoida 0.06 Ostracoda (Naqvi et al.1985)
NOEC values to crustaceans, mg/l	0.0035 rpd, schr, Daphnia magna (Macek et al. 1976c)

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LC50 values to fishes, mg/l	0.21–0.042	96hr, Salmo gairdneri (Macek et al. 1967)
	0.019	48hr, Lepomis macrochirus
	0.011	Salmo gairdneri (Edwards 1977)
	0.19	96hr, srv, act, Cyprinodon variagetus (Parrish et al. 1978)
	0.01–0.09	Salmo gairdneri
	0.047	Lepomis macrochirus
	0.093	Pimephales promelas (Kenaga 1979)
	1	48hr, Cyprinus carpio
	0.85	Carassius auratus (Hashimoto & Nishiuchi 1981)
LOEC values to fishes, mg/l	0.005	srv, rpd, chr, Pimephales promelas (Macek et al. 1976c)
	0.005	Cyprinodon variegetus (Parrish et al.1977)
	0.005	rpd, chr, C.variegetus (Parrish 1978)
	0.018	srv, grw, chr, Cyprinodon variagetus (Ward & Parrish 1980)
NOEC values to fishes, mg/l	0.002	srv, rpd, chr, Pimephales promelas (Macek et al. 1976c)
	0.001	rpd, chr, Cyprinodon variagetus (Parrish 1978)

1977 • Triforin 26644-46-2

LC50 values to fishes, mg/l	> 1000	96hr, Salmo gairdneri Lepomis macrochirus (Pesticide Manual 1983)

1978 • Trihexylsilanol 60782-58-3

Sumformula of the chemical	C18H40OSi	
Water solubility, mg/l	0.00003	(MITI 1992)
Melting point, °C	< -10	(MITI 1992)
Boiling point, °C	> 300	(MITI 1992)
Log octanol/water coefficient, log Pow	> 6.39	(MITI 1992)
Bioconcentration factor, fishes	5.6–22	6w, Cyprinus carpio, conc 0.25
	11–50	6w, Cyprinus carpio, conc 0.025 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 500	48hr, Oryzias latipes (MITI 1992)

1979 • 2,4,6-Trihydroxy-1,3-diazine 67-52-7

Sumformula of the chemical	C4H4N2O3	
EINECS-number	2006580	
Melting point, °C	245	(MITI 1992)

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Total degradation in water	Biodegradation: 76% (NH3) by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

1980 • 1,3,5-Trihydroxybenzene 108-73-6

Synonyms	1,3,5-Benzenetriol
LC50 values to fish, mg/l	630 48hr, Carassius auratus (McKee & Wolf 1963)

1981 • Triisobutylene 7756-94-7

Sumformula of the chemical	C12H24
Water solubility, mg/l	110 (MITI 1992)
Boiling point, °C	177 (MITI 1992)
Log octanol/water coefficient, log Pow	5 ± 0.4 (MITI 1992)
Total degradation in water	Biodegradation (Closed Bottle test): 1% by BOD period: 28d substance: 7.7 mg/l sludge: 2 mg (AS)/l 3% by BOD period: 28d substance: 1.5 mg/l sludge: 2 mg (AS)/l (MITI 1992).
Bioconcentration factor, fishes	1360–3150 8w, Cyprinus carpio, conc 0.5 mg/l 1100–2380 8w, Cyprinus carpio, conc 0.5 mg/l 990–4290 8w, Cyprinus carpio, conc 0.05 mg/l 870–2670 8w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
LC50 values to fishes, mg/l	1000 48hr, Oryzias latipes (MITI 1992)

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1982 • Triisopropylnaphthalene 35860-37-8

Water solubility, mg/l	0.01 (MITI 1992)
Boiling point, °C	328 (MITI 1992)
Log octanol/water coefficient, log Pow	6.03 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).

Bioconcentration factor, fishes	1520–11000 12w, Cyprinus carpio, conc 0.05 mg/l 2860–14500 12w, Cyprinus carpio, conc 0.005 mg/l 2320–7600 12w, Cyprinus carpio, conc 0.001 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be accumulated on a medium level (Anon. 1987).
LC50 values to fishes, mg/l	105 48hr, Oryzias latipes (MITI 1992)

1983 • Trimellitic anhydride 552-30-7

Sumformula of the chemical	C9H4O5
Melting point, °C	168–168.5 (MITI 1992)
Boiling point, °C	240–245 14 mmHg (MITI 1992)
Total degradation in water	Biodegradation: 89–101% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

1984 • Trimethyl amine 75-50-3

Sumformula of the chemical	C3H9N
EINECS-number	2008750
Water solubility, mg/l	410000 (MITI 1992)
Melting point, °C	-117 (MITI 1992)
Boiling point, °C	2.9 (MITI 1992)
Total degradation in water	Biodegradation: 92% by BOD (NH3) 66% by BOD (NO2) period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

1985 • Trimethyl phosphate 512-56-1

Sumformula of the chemical	C3H9O4P
Water solubility, mg/l	> 10000 (MITI 1992)
Boiling point, °C	197 (MITI 1992)
Log octanol/water coefficient, log Pow	-0.46 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

Bioconcentration factor, fishes	0.2–0.4 6w, Cyprinus carpio, conc 2 mg/l < 1.4 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	> 1000 48hr, Oryzias latipes (MITI 1992)

1986 • 2,4,6-Trimethyl-1,3,5-trioxane 123-63-7

Synonyms	Para-acetaldehyde
Sumformula of the chemical	C6H12O3
EINECS-number	2046398
Water solubility, mg/l	125 (MITI 1992)
Melting point, °C	12.6 (MITI 1992)
Boiling point, °C	124 (MITI 1992)
Total degradation in water	Biodegradation: 12.0% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).
Bioconcentration factor, fishes	< 0.3 6w, Cyprinus carpio, conc 2 mg/l < 3.0 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	1000 48hr, Oryzias latipes (MITI 1992)

1987 • 2,2,4-Trimethyl-1,3-pentanediol 144-19-4

Sumformula of the chemical	C8H18O2
EINECS-number	2056191
Water solubility, mg/l	35000 (MITI 1992)
Melting point, °C	50–53 (MITI 1992)
Log octanol/water coefficient, log Pow	1.24 (MITI 1992)
Total degradation in water	Biodegradation: 4–82% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	0.6–0.8 6w, Cyprinus carpio, conc 1 mg/l < 1.0 6w, Cyprinus carpio, conc 0.1 mg/l (MITI 1992)
LC50 values to fishes, mg/l	837 48hr, Oryzias latipes (MITI 1992)

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1988 • 2,4,4-Trimethyl-1-pentene 107-39-1

Water solubility, mg/l	< 10 mg/l	(MITI 1992)
Boiling point, °C	101.44	(MITI 1992)
Log octanol/water coefficient, log Pow	1.55	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 1.4 mg/l sludge: 2 mg/l 0% by BOD period 28d substance: 7.2 mg/l sludge: 2 mg/l (MITI 1992).	
Bioconcentration factor, fishes	358–729 350–868	8w, Cyprinus carpio, conc 0.025 mg/l 8w, Cyprinus carpio, conc 0.0025 mg/l (MITI 1992)
LC50 values to fishes, mg/l	3 2.15	24hr, Carassius auratus (Anon. 1975) 48hr, Oryzias latipes (MITI 1992)

1989 • N,N, N-Trimethyl-2-hydroxyethyl ammoniumchloride 67-48-1

Sumformula of the chemical	C5H14NO.Cl
EINECS-number	2006554
Total degradation in water	Biodegradation: 93.5% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

1990 • 2,2,4-Trimethyl-3-hydroxypentyl isobutyrate 77-68-9

Sumformula of the chemical	C12H24O3	
EINECS-number	2010492	
Melting point, °C	-57	(MITI 1992)
Boiling point, °C	248	(MITI 1992)
Total degradation in water	Biodegradation: 93–99% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

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1991 • 1,2,3-Trimethylbenzene 526-73-8

Sumformula of the chemical	C9H12	
Water solubility, mg/l	< 10	(MITI 1992)
Melting point, °C	-25.4	(MITI 1992)
Boiling point, °C	176.1	(MITI 1992)
Log octanol/water coefficient, log Pow	3.76 3.6	(MITI 1992) (Schwarzenbach & Westall 1981)
Log soil sorption coefficient, log Kom	2.8 2.77	observed (Sabljic 1987) calculated (Sabljic 1987)
Henry's law constant, Pa x m³/mol	364	calc (Yaws et al. 1991)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	133–217 136–259	8w, Cyprinus carpio, conc 0.15 mg/l 8w, Cyprinus carpio, conc 0.015 mg/l (MITI 1992)
LC50 values to fishes, mg/l	7	48hr, Oryzias latipes (MITI 1992)

1992 • 1,2,4-Trimethylbenzene 95-63-6

Water solubility, mg/l	< 10	(MITI 1992)
Boiling point, °C	169–171	(MITI 1992)
Log octanol/water coefficient, log Pow	3.63	(Sangster 1989)
Henry's law constant, Pa x m³/mol	570.8	calc. (Yaws et al. 1991)
Total degradation in water	Biodegradation: 4–18% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).	
Bioconcentration factor, fishes	33–275 31–207	8w, Cyprinus carpio, conc 0.2 mg/l 8w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon.1987).	
LC50 values to fishes, mg/l	18	48hr, Oryzias latipes (MITI 1992)

1993 • Trimethylene glycol 504-63-2

Synonyms	1,3-Propanediol

Chemical oxygen demand, g 02/g	1.64	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	0.18	5 days (Bridie et al. 1979)
LC50 values to fishes, mg/l	> 5000	Carassius auratus (Bridie et al. 1979)

1994 • Trimethyllead chloride 1520-78-1

LC50 values to fishes, mg/l	25 32	96hr, Platichthys flesus 96hr, Salmo gairdneri (Maddock & Taylor 1977)
Other information about water organisms	LC50 (96hr) 0.50 mg/l, mussel (Maddock & Taylor 1977).	

1995 • Trimethylolpropane 77-99-6

LC50 values to crustaceans, mg/l	5250	96hr, 10 °C, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	> 10000	96hr, 10 °C, Alburnus alburnus (Linden et al. 1979)

1996 • 2,4,6-Trimethylphenol 527-60-6

Sumformula of the chemical	C9H12O	
Water solubility, mg/l	1200	(MITI 1992)
Melting point, °C	73	(MITI 1992)
Boiling point, °C	220	(MITI 1992)
Log octanol/water coefficient, log Pow	2.8	(MITI 1992)
Total degradation in water	Biodegradation: 7% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	6.5–10 < 2.7–8.1	6w, Cyprinus carpio, conc 0.2 mg/l 6w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
LC50 values to fishes, mg/l	14.3	48hr, Oryzias latipes (MITI 1992)

1997 • 2,4,6-Trinitro-5-tert-butyl-1,3-xylene 81-15-2

Sumformula of the chemical	C12H15N3O6	
EINECS-number	2013294	
Water solubility, mg/l	2	(MITI 1992)
Melting point, °C	103–105	(MITI 1992)
Log octanol/water coefficient, log Pow	5.2	(MITI 1992)

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Total degradation in water	Biodegradation: 0–6% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	640–5820 1440–6740	10w, Cyprinus carpio, conc 0.01 mg/l 10w, Cyprinus carpio, conc 0.001 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be accumulated on a medium level (Anon. 1987).	
LC50 values to fishes, mg/l	3.75	48hr, Oryzias latipes (MITI 1992)

1998 • 1,3,5-Trinitrobenzene 99-35-4

Synonyms	sym-Trinitrobenzene	
Use	In explosives.	
Molecular weight	213.12	
LD50 values to mammals in oral exposure, mg/kg	450	orl-rat (Lewis & Sweet 1984)
LOEC values to algae, mg/l	0.1	rpd, 5d, Selenastrum capricornutum (van der Shalie 1983)
EC50 values to crustaceans, mg/l	2.7 3	mbt,48hr, Daphnia magna (Pearson et al. 1979) 48hr, rpd, Daphnia magna (van der Shalie 1981)
LOEC values to crustaceans, mg/l	0.75	rpd,21d, Daphnia magna (van der Shalie 198)
LC50 values to fishes, mg/l	0.52 1.03	96hr, Salmo gairdneri (van der Shalie 1983) 96hr, Pimephales promelas (Pearson et al. 1979)
LOEC values to fishes, mg/l	0.17	phy, 71d, Salmo gairdneri (van der Shalie 1983)

1999 • Trinitrobenzene-aniline complex 3101-79-9

Other information about mammals	LDfr = 75.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

2000 • 2,4,6-Trinitroresorsinol 82-71-3

Synonyms	Styphnic acid 2,4,6-Trinitro-1,3-benzenediol	
State and appearance	Yellow crystals.	
Molecular weight	245.12	
Melting point, °C	179–180	
LOEC values to algae, mg/l	0.32	rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to fishes, mg/l	2.6	96hr, Pimephales promelas (Verschueren 1983)
EC50 values to fishes, mg/l	0.46	bhv,96hr, Pimephales promelas (Verschueren 1983)

2001 • 2,4,6-Trinitrotoluene 118-96-7

Synonyms	TNT	
Use	Explosive, intermediate in dyestuffs and photographic chemicals.	
State and appearance	Colourless crystals.	
Molecular weight	227.15	
Water solubility, mg/l	200	15 °C
Melting point, °C	80.7	
Other physicochemical properties	240 °C, explodes.	
LD50 values to mammals in oral exposure, mg/kg	795 660	orl-rat orl-mus (Lewis & Sweet 1984)
LDLo values to mammals in oral exposure, mg/kg	500	orl-rbt (Lewis & Sweet 1984)
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): > 100 mg/l (Bringmann & Kühn 1980a).	
LOEC values to algae, mg/l	1.6	rpd, schr, Scenedesmus quadricauda (Bringmann & Kühn 1980a)
EC50 values to crustaceans, mg/l	11.9	mbt, 48hr, Daphnia magna (Pearson et al. 1979)
LC50 values to fishes, mg/l	2.4 2.58 2.6	96hr, Pimephales promelas (Pearson et al. 1979) 96hr, Pimephales promelas (Smock et al. 1976) 96hr, Pimephales promelas (Lockhart et al. 1975)
EC50 values to fishes, mg/l	0.46	bhv,96hr, Pimephales promelas (Lockhart et al. 1975)
Other information about water organisms	LOEC 1.6 mg/l, rpd, schr, Entosiphon sulcatum (Bringmann & Kühn 1980a). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 1.6 mg/l protozoa (Entosiphon sulcatum): 1.6 mg/l (Bringmann & Kühn 1980a).	

2002 • Trioctyl amine 1116-76-3

Sumformula of the chemical	C24H51N	
Water solubility, mg/l	0.05	(MITI 1992)
Melting point, °C	-34	(MITI 1992)
Boiling point, °C	365	(MITI 1992)
Log octanol/water coefficient, log Pow	> 6.3	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).	
Bioconcentration factor, fishes	23–101 25–143	8w, Cyprinus carpio, conc 0.05 mg/l 8w, Cyprinus carpio, conc 0.005 mg/l (MITI 1992)

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Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	5.1	48hr, Oryzias latipes (MITI 1992)

2003 • 1,3,5-Trioxane 110-88-3

Synonyms	s-Trioxane Formaldehyde, trimer	
Sumformula of the chemical	C3H6O3	
EINECS–number	2038125	
State and appearance	Crystalline solid.	
Odour	Characteristic chloroform-like odour.	
Molecular weight	90.08	
Water solubility, mg/l	172	17.2/100 ml, 18–25 °C (HSDB 1995)
Melting point, °C	64	(HSDB 1995)
Boiling point, °C	114.5	(HSDB 1995)
Other physicochemical properties	Easily soluble in alcohols, ketones, ether, acetone, organic solvents, chlorinated and aromatic hydrocarbons. Slightly soluble in pentane, petroleum ether, lower paraffins (HSDB 1995).	
EC50 values to crustaceans, mg/l	15200	48hr, imb, Daphnia magna (AQUIRE 1995)
LC50 values to fishes, mg/l	16350 5950	96hr, Cyprinodon variegatus 96hr, Pimephales promelas

2004 • Triphenyl amine 603-34-9

Sumformula of the chemical	C18H15N	
pKa	-5	(Sangster 1989)
Log octanol/water coefficient, log Pow	5.74 5.74	(Anon. 1986) (Sangster 1989)

2005 • Triphenyl phosphate 115-86-6

Use	Solvent, plasticiser.	
Molecular weight	326	
Melting point, °C	49.9	(MITI 1992)
Boiling point, °C	370	760 mmHg (MITI 1992)
Log octanol/water coefficient, log Pow	4.6	(Anon. 1988)
Mobility	Equilibrium distribution: air water solid	 *mass %* 0.77 13.96 85.28 (Anon. 1988).

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Total degradation in water	Biodegradation: 83–94% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
LC50 values to fishes, mg/l	290 96hr, Lepomis macrochirus 95 96hr, Menidia audens (Dawson et al. 1977) 1.2 96hr, Oryzias latipes 0.7 96hr, Carassius auratus (Sasaki et al. 1981)

2006 • Triphenylchlorosilane 76-86-8

Sumformula of the chemical	C18H15ClSi
EINECS-number	2009890
Melting point, °C	90–93 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

2007 • Triphenylsilanol 791-31-1

Sumformula of the chemical	C18H16OSi
Bioconcentration factor, fishes	297–667 8w, Cyprinus carpio, conc 0.5 mg/l 491–1050 8w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 250 48hr, Oryzias latipes (MITI 1992)

2008 • Triphenyltin acetate 900-95-8

Synonyms	Fentin acetate
Use	Fungicide.
Molecular weight	409.07
LD50 values to mammals in oral exposure, mg/kg	125 orl-rat 30 orl-rbt (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	450 skn-rat (Lewis & Sweet 1984)
LDLo values to mammals in oral exposure, mg/kg	10 orl-gpg (Lewis & Sweet 1984)
Other information about mammals	LDfr = 75.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

LD50 values to birds in oral exposure, mg/kg	100	orl-qal (Lewis & Sweet 1984)
	100	orl-Agelaius phoeniceus
	100–117	orl-Coturnix coturnix (Schafer et al. 1983)
Effects on arthropods	Chironomus riparius, LC50: 1 d, 0.070 mg/l; 2 d, 0.050 mg/l (Cotta-Ramusino & Doci 1987).	
EC50 values to algae, mg/l	0.00086	rpd,72hr, Skeletonema costatum (Walsh et al. 1985)
LC50 values to crustaceans, mg/l	0.023	act, Daphnia pulex (Hashimoto & Nichiuchi 1981)
	3	1d, Asellus aquaticus
	1.1	2d, Asellus aquaticus (Cotta-Ramusino & Doci 1987)
LC50 values to fishes, mg/l	0.064	48hr, Cyprinus carpio
	0.062	48hr, Carassius auratus (Hashimoto & Nihiuchi 1981)
	0.676	1d, Carassius auratus
	0.62	2d, Carassius auratus (Cotta-Ramusino & Doci 1987)

2009 • Triphenyltin chloride 639-58-7

Synonyms	Chlorotriphenylstannane	
Molecular weight	385.47	
LD50 values to mammals in oral exposure, mg/kg	135	orl-rat
	18	orl-mus (Lewis & Sweet 1984)
LC50 values to algae, mg/l	0.04	pht, act, Selenastrum quadricauda (Wong et al. 1982)
EC50 values to algae, mg/l	0.00092	rpd,72hr, Skeletonema costatum (Walsh et al. 1985)

2010 • Triphenyltin fluoride 379-52-2

Synonyms	Fluorotriphenylstannane	
Other information about bioaccumulation	Confirmed to be accumulated on a medium level (Anon. 1987).	
LC50 values to crustaceans, mg/l	0.008	96hr, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	0.4	96hr, Alburnus alburnus (Linden et al. 1979)

2011 • Triphenyltin hydroxide 76-87-9

Synonyms	TPTH Dowco 186 Fentin hydroxide Hydroxytriphenylstannane Hydroxytriphenyltin Triphenyltin oxide
Sumformula of the chemical	C18H16OSn

Products containing the chemical	Erithane
Use	Fungicide.
State and appearance	White odourless powder.
Molecular weight	367.03
Water solubility, mg/l	0.4 (MITI 1992)
Melting point, °C	118–120 117–119 (MITI 1992)
Log octanol/water coefficient, log Pow	3.66 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOd period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	1360–6040 10w, Cyprinus carpio, conc 0.001 mg/l 617–7100 10w, Cyprinus carpio, conc 0.0001 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be accumulated on a medium level (Anon. 1987).
LD50 values to mammals in oral exposure, mg/kg	46 orl-rat (Lewis & Sweet 1984) 245 orl-mus (Sweet 1987)
LDLo values to mammals in non-oral exposure, mg/kg	8.5 ipr-mus 100 ipr-rat (Sweet 1987)
TDLo values to mammals in oral exposure, mg/kg	105 8-14d preg., orl-rat effects on embryo or fetus 140 1-7d preg., orl-rat effects on fertility 105 8-14d preg., orl-rat effects on fertility (Sweet 1987)
Other information about mammals	LDfr = 75.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).
Carcinogenicity	NCI carcinogenesis bioassay completed: results negative; mus, rat (Lewis & Sweet 1984).
LD50 values to birds in oral exposure, mg/kg	> 100 orl-Agelaius phoeniceus (Schafer et al. 1983)
EC50 values to algae, mg/l	0.00059 rpd,72hr, Skeletonema costatum (Walsh et al. 1985)
LC50 values to fishes, mg/l	0.042 48hr, Rasbora heteromorpha 0.015 96hr, Salmo gairdneri (Tooby et al. 1975) 0.0529 48hr, Oryzias latipes (MITI 1992)

2012 • Tripropyltin acetate 3267-78-5

Other information about mammals	LDfr = 62.5 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

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2013 • Tripropyltin chloride 2279-76-7

LD50 values to birds in oral exposure, mg/kg	> 79	orl-Agelaius phoeniceus (Schafer et al. 1983)
LC50 values to algae, mg/l	0.02	pht, Ankistrodesmus falcatus (Wong et al. 1982)

2014 • Tris(1-chloro-2-propyl)phosphate 13674-84-5

Sumformula of the chemical	C9H18O4PCl3	
Water solubility, mg/l	1200	(MITI 1992)
Melting point, °C	-40	(MITI 1992)
Boiling point, °C	> 270	(MITI 1992)
Log octanol/water coefficient, log Pow	2.59	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	0.8–2.8 < 1.9–4.6	6w, Cyprinus carpio, conc 0.2 mg/l 6w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
LC50 values to fishes, mg/l	54.2	48hr, Oryzias latipes (MITI 1992)

2015 • Tris(1-nitroso-2-naphthol)cobalt 26076-28-8

Water solubility, mg/l	< 10	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	6.8–18 28–96	8w, Cyprinus carpio, conc 0.048 mg/l 8w, Cyprinus carpio, conc 0.0048 mg/l (MITI 1992)
LC50 values to fishes, mg/l	4.68	48hr, Oryzias latipes (MITI 1992)

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2016 • 1,3,5-Tris(2'-hydroxyethyl)-isocyanuric acid 839-90-7

Sumformula of the chemical	C9H15N3O6	
Melting point, °C	133	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	

Bioconcentration factor, fishes	< 0.16 < 1.6	6w, Cyprinus carpio, conc 2.5 mg/l 6w, Cyprinus carpio, conc 0.25 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	1000	48hr, Oryzias latipes (MITI 1992)

2017 • Tris(2,3-dibromopropyl)phosphate 126-72-7

Melting point, °C	-8	(MITI 1992)
Boiling point, °C	260	(MITI 1992)
Log octanol/water coefficient, log Pow	4.98 1.75	(Mackay 1982) (MITI 1992)
Total degradation in water	Biodegradation: 1.8% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.7–1.9 < 2.2–4.3	6w, Cyprinus carpio, conc 0.1 mg/l 6w, Cyprinus carpio, conc 0.03 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
EC50 values to algae, mg/l	3.1	96hr, grw, Scenedesmus subspicatus (Geyer et al. 1985)
LC50 values to fishes, mg/l	0.24 1.45 87	eggs, 96hr, Salmo gairdneri 96hr, Salmo gairdneri (Sitthichaikasem 1978) 48hr, Oryzias latipes (MITI 1992)

2018 • Tris(2-chloroethyl)phosphate 115-96-8

Sumformula of the chemical	C6H12Cl3O4P	
EINECS-number	2041185	
Water solubility, mg/l	> 1000	(MITI 1992)
Melting point, °C	< -20	(MITI 1992)
Boiling point, °C	210–220	30 mmHg (MITI 1992)
Log octanol/water coefficient, log Pow	1.44	(MITI 1992)
Total degradation in water	Biodegradation: 4% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	0.6–0.8 < 1.2–5.1	6w, Cyprinus carpio, conc 1.0 mg/l 6w, Cyprinus carpio, conc 5.1 mg/l (MITI 1992)

Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	300	48hr, Oryzias latipes (MITI 1992)

2019 • Tris(2-ethylhexyl)benzene-tricarboxylate 3319-31-1

Sumformula of the chemical	C33H54O6	
Water solubility, mg/l	100	(MITI 1992)
Total degradation in water	Biodegradation: 4.2% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.1–0.23 < 1–2.7	6w, Cyprinus carpio, conc 2 mg/l 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	> 1000	48hr, Oryzias latipes (MITI 1992)

2020 • Tris(2-ethylhexyl)phosphate 78-42-2

Sumformula of the chemical	C24H51O4P	
EINECS-number	2011166	
Water solubility, mg/l	2	(MITI 1992)
Log octanol/water coefficient, log Pow	5.04	(MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	2.4–6.5 9.2–22	6w, Cyprinus carpio, conc 2 mg/l 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 500	48hr, Oryzias latipes (MITI 1992)

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2021 • Tris(2-hydroxypropyl)amine 122-20-3

Synonyms	1,1',1''-Nitrilotris-2-propanol	
Sumformula of the chemical	C9H21NO3	
EINECS-number	2045284	
Melting point, °C	58	(MITI 1992)
Boiling point, °C	305	(760 mmHg) (MITI 1992)

Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.06 < 0.57	6w, Cyprinus carpio, conc 2.5 mg/l 6w, Cyprinus carpio, conc 0.25 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 1000	48hr, Oryzias latipes (MITI 1992)

2022 • Tris(p-isopropylphenyl)phosphate 26967-76-0

Sumformula of the chemical	C27H33O4P	
Water solubility, mg/l	< 0.1	(MITI 1992)
Melting point, °C	-20	(MITI 1992)
Boiling point, °C	305	2 mmHg (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	6.9–17 20–43	6w, Cyprinus carpio, conc 2 mg/l 6w, Cyprinus carpio, conc 0.2 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 240	48hr, Oryzias latipes (MITI 1992)

2023 • Tris(phenyl, monomethylphenyl, dimethylphenyl, ethylphenyl, nonylphenyl)phosphate 10113-28-7

Water solubility, mg/l	< 10	(MITI 1992)
Melting point, °C	< -20	(MITI 1992)
Boiling point, °C	240–260	2 mmHg (MITI 1992)
Total degradation in water	Biodegradation: 0–40% by BOD period: 28d substance: 30 mg/l sludge: 100 mg/l (MITI 1992).	
Bioconcentration factor, fishes	35–282 63–269 44–165 302–1130 372–742 279–640	8w, Cyprinus carpio, conc 0.2 mg/l 8w, Cyprinus carpio, conc 0.2 mg/l 8w, Cyprinus carpio, conc 0.2 mg/l 8w, Cyprinus carpio, conc 0.02 mg/l 8w, Cyprinus carpio, conc 0.02 mg/l 8w, Cyprinus carpio, conc 0.02 mg/l (MITI 1992)
LC50 values to fishes, mg/l	> 200	48hr, Oryzias latipes (MITI 1992)

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2024 • Tris(polyoxypropylene)glyceryl ether 25791-96-2
(average molecular weight ca. 3000)

Sumformula of the chemical	(C3H60)n.(C3H60)n.(C3H60)n.C3H803
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be non-biodegradable (Anon. 1987).
Bioconcentration factor, fishes	< 0.7–2.2 6w, Cyprinus carpio, conc 6 mg/l < 7 6w, Cyprinus carpio, conc 0.6 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	630 48hr, Oryzias latipes (MITI 1992)

2025 • Tris-(tributyltin) phosphate 13435-05-7

Other information about mammals	LDfr = 100 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

2026 • Tristearylphosphite 2082-80-6

Synonyms	Phosphorous acid, trioctadecyl ester
Sumformula of the chemical	C54H11103P
EINECS-number	2182176
Water solubility, mg/l	52 (MITI 1992)
Melting point, °C	44 (MITI 1992)
Total degradation in water	Biodegradation: 63–70% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

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2027 • Triton X-405 9002-93-1

Other information about water organisms	100% mortality: Poteriochromonas malhamensis, 3 d, 124.3 mg/l (Roderer 1987).

2028 • N-Tritylmorpholine 1420-06-0

LC50 values to fishes, mg/l	0.083 48hr, Salmo trutta m. lacustris (Matthiessen 1977)

2029 • U 15766

672-06-0

Other information about mammals	ALD = 94.0 mg/kg, act, orl, deer mouse; LDfr = 37.5 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).

2030 • Undecanol

112-42-5

Synonyms	1-Undecanol	
LC50 values to crustaceans, mg/l	1.4	96hr, 21 °C, Nitocra spinipes (Linden et al. 1979)
LC50 values to fishes, mg/l	1.04	96hr, Pimephales promelas (Veith et al. 1983)
	4.6	96hr, 10 °C, Alburnus alburnus (Linden et al. 1979)

2031 • Uranium and uranium compounds

7440-61-1

LC50 values to crustaceans, mg/l	6	U(VI), 48hr, Daphnia magna (Poston et al. 1984)
LOEC values to crustaceans, mg/l	0.5	U(VI), rpd, chr, Daphnia magna (Poston et al. 1984)

2032 • Urea

57-13-6

Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): > 10000 mg/l (Bringmann & Kühn 1980a).
Other information about water organisms	LOEC 29 mg/l, rpd, schr, Entosiphon sulcatum (Bringmann & Kühn 1980a). Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): > 10000 mg/l protozoa (Entosiphon sulcatum): 29 mg/l (Bringmann & Kühn 1980a).

2033 • Valeric acid

109-52-4

Synonyms	Pentanoic acid Butanecarboxylic acid 1-Butanecarboxylic acid n-Pentanoic acid Propylacetic acid Valerianic acid n-Valeric acid	
Sumformula of the chemical	C5H10O2	
pKa	4.83	(Sangster 1989)
Log octanol/water coefficient, log Pow	1.39	(Sangster 1989)
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	
LD50 values to mammals in oral exposure, mg/kg	600	orl-mus (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	1290 3590	ivn-mus scu-mus (Sweet 1987)

UVW

LCLo values to mammals in inhalation exposure, mg/kg	4100	2hr, ihl-mus (Sweet 1987)
LC50 values to crustaceans, mg/l	45	48hr, Daphnia magna (Freeman 1953)
LC50 values to fishes, mg/l	77	96hr, Pimephales promelas (Vincent et al. 1976)

2034 • Vamidothion 2275-23-2

Use	Acaricide; insecticide.	
LC50 values to crustaceans, mg/l	> 10	act, Daphnia pulex (Nishiuchi & Hashimoto 1967)
LC50 values to fishes, mg/l	> 40	48hr, Cyprinus carpio (Nishiuchi & Hashimoto 1967)

2035 • Vanadium and vanadium compounds 7440-62-2

LC50 values to crustaceans, mg/l	2 3.4–4.8	23d, rpd, Daphnia magna 48hr, Daphnia magna (Beusen & Neven 1987)
EC50 values to crustaceans, mg/l	2.9–4.0 0.8–2.6	48hr, srv, Daphnia magna (Beusen & Neven 1987) 48hr, srv, Daphnia magna (Beusen & Neven 1987)
LC50 values to fishes, mg/l	0.17 8.0–19.4 2.9–5.3 14.2–17.1 6.1–10.2	28d, Salmo gairdneri (Birge et al. 1980) 48hr, Branchydanio rerio 96hr, Branchydanio rerio (Beusen & Neven 1987) 48hr, Poecilia reticulata 96hr, Poecilia reticulata (Beusen & Neven 1978)
LOEC values to fishes, mg/l	0.17	srv, grw, chr, flag fish (Holdway & Spraque 1979)
NOEC values to fishes, mg/l	0.04	srv, grw, chr, flag fish (Holdway & Spraque 1979)

2036 • Vanadium pentoxide 1314-62-1

LC50 values to fishes, mg/l	11 15 14 12 4 2	2d, Salvelinus fontinalis 4d, Salvelinus fontinalis 6d, Salvelinus fontinalis 8d, Salvelinus fontinalis 10d, Salvelinus fontinalis 30d, Salvelinus fontinalis (Ernst & Garside 1987)

2037 • Vapan 137-42-8

Effects on physiology on aquatic organisms	Salmo gairdneri, 0.070 mg/l, 4 d, change in enzyme activity (Castren & Oikari 1987).

2038 • Vat Blue-1

482-89-3

Sumformula of the chemical	C16H10N2O2	
Total degradation in water	Biodegradation: 0% by BOD period: 14d substance: 100 m, g/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	< 0.26–4.5 < 2.5	6w, Cyprinus carpio, conc 0.4 mg/l 6w, Cyprinus carpio, conc 0.04 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	> 100	48hr, Oryzias latipes (MITI 1992)

2039 • Veratrol

91-16-7

Synonyms	1,2-Dimethoxybenzene	
Sumformula of the chemical	C8H10O2	
EINECS-number	2020453	
Water solubility, mg/l	> 1000	(MITI 1992)
Total degradation in water	Biodegradation: 95–97% by BOD period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).	

2040 • Versatic 10

52627-73-3

LC50 values to fishes, mg/l	80	96hr, Carassius auratus (Anon. 1975)
	30	96hr, Salmo gairdneri (Dave & Lidman 1978)

2041 • Vinclozolin

50471-44-8

Use	Active ingredient in fungicides.	
LC50 values to fishes, mg/l	32.5 52.5	96hr, Poecilia reticulata 96hr, Salmo salar (Pesticide Manual 1983)

2042 • 4-Vinyl-1-cyclohexene

100-40-3

Sumformula of the chemical	C8H12	
EINECS-number	2028489	
Water solubility, mg/l	50	(MITI 1992)

Log octanol/water coefficient, log Pow	3.93 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	83–211 8w, Cyprinus carpio, conc 0.1 mg/l 110–208 8w, Cyprinus carpio, conc 0.01 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LC50 values to fishes, mg/l	17 48hr, Oryzias latipes (MITI 1992)

2043 • Vinylacetate 108-05-4

Synonyms	1-Acetoxyethylene Vinyl acetate
Sumformula of the chemical	C4H6O2
Use	Solvent.
Odour	Quality: sour, sharp Hedonic tone: unpleasant Threshold odour concentration absolute: 0.12 ppm 50% recognition: 0.40 ppm 100% recognition: 0.55 ppm Odour index 100% recognition: 220 000 (Hellman & Small 1974).
Molecular weight	86.09
Vapour pressure, mmHg	85 at 20 °C (Weber et al. 1981)
Water solubility, mg/l	20000 at 20 °C (Merck Index 1983) 26000 (MITI 1992)
Melting point, °C	-93.2 (Howard I 1990) < -84 (MITI 1992)
Boiling point, °C	72–73 (MITI 1992)
Log octanol/water coefficient, log Pow	0.73 (Hansch & Leo 1985) 0.73 (Sangster 1989)
Henry's law constant, Pa x m³/mol	48.7 at 20 °C, calc. (Howard I 1990)
Volatilization	The Henry's Law constant suggests that volatilization from environmental waters can be significant. (Lyman et al. 1982) The volatilization half-life from a model river (1 m deep flowing 1 m/sec with a wind speed of 3 m/sec) can be estimated to be 4.4hr. (Lyman et al. 1982) The volatilization half-life from an environmental pond can be estimated to be 2.1 days (USEPA 1987)
Adsorption/desorption	Based on the water solubility and the log Kow, the Koc of vinyl acetate can be estimated to range from 19 to 59 from regression-derived equation (Lyman et al. 1982).

Mobility	The estimated Koc values are indicative of very high to high soil mobility (Swann et al. 1983). Vinyl acetate readily polymerizes, therefore, if vinyl acetate is released to the environment in a spill situation, significant polymerization may occur (Howard 1989).
Photochemical degradation in air	Vapour-phase vinyl acetate is degraded rabidly in the atmosphere by reaction with photochemically produced hydoxyl radicals, estimated half-life of 14.6 hours in a average atmosphere (Atkinson 1987).
Photochemical degradation in water	The half-lifes for olefinic structures in sunlit natural waters are about 13 and 18 days with respect to reaction via hydroxyl radicals and singlet oxygen. Vinyl avetate does not absorb UV light significantly above 250 nm in ethanol solvent and, therefore, it should not be susceptible to direct sunlight photolysis (Mill & Mabey 1985) (Daniels 1983).
Hydrolysis in water	The aqueous hydrolysis half-life of vinyl acetate at 25 °C and pH 7 has been reported to 7.3 days. Hydrolysis rates will increase as the soil becomes more alkaline (Mabey & Mill 1978). The hydrolysis rate at pH 4.4 has been reported to be minimal (Daniels 1983).
Total degradation in water	Biodegradation: 82–98% by BOD period 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Other information about degradation	A 5-day 42% BODT in marine water and a 5-day 51.3% BODT using a sewage inocula (Takemoto 1981). A 62% BODT in 5 days and a 72% BODT in 20 days using an acclimated sewage inoculum; 51 and 69% BODTs in 5 and 15 days, respectively, in marine water containing a syntetic sewage seed (Price et al. 1974). CO2 evolutions of 27 and 49% over 19 and 38 days incubation, respectively, using non-acclimated sewage inocula; a 58% CO2 evolution in 22 days using an acclimated sewage inocula (Pahren & Bloodgood 1961). CO2 evolution of 42% in 10 days using an acclimated sewage inocula (Ludzack & Ettinger 1960). A 100% degradation after a 3-day lag period using the Hungate Serum Bottle technique (aerobic conditons) and enriched methane cultures (Chou et al. 1979).
LDLo values to mammals in oral exposure, mg/kg	500 orl-rat
Effects on microorganisms	Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida): 6 mg/l (Bringmann & Kühn 1980a).
LOEC values to algae, mg/l	35 rpd, schr, Microcystis aeruginosa (Bringmann & Kühn 1976)
LC50 values to fishes, mg/l	18 96hr, Lepomis macrochirus 19 96hr, Pimephales promelas (Pickering & Henderson 1966)
Other information about water organisms	Toxicity threshold (cell multiplication inhibition test): green algae (Scenedesmus quadricauda): 370 mg/l protozoa (Entosiphon sulcatum): 81 mg/l (Bringmann & Kühn 1980a).

UVW

2044 • Vinylchloride

75-01-4

Synonyms	Chloroethene Chloroethylene Vinyl chloride

Sumformula of the chemical	C_2H_3Cl	
State and appearance	Colourless gas.	
Molecular weight	62.5	
Vapour pressure, mmHg	2660	25 °C (Riddick et al. 1986)
Water solubility, mg/l	1100 2763	25 °C 25 °C (Horvath 1982)
Melting point, °C	-153– -160 -153.8	
Boiling point, °C	-13.9 -13.37	
Log octanol/water coefficient, log Pow	1.38	calc. (Hansch & Leo 1985)
Henry's law constant, Pa x m³/mol	1084	(Hine & Mookerjee 1975)
Volatilization	Based on Henry's Law constant, a half-life of 0.805hr was calculated for evaporation from a river 1 m deep with a current of 3 m/sec and with a wind velocity of 3 m/sec. (Lyman et al. 1982) Due to high Henry's Law constant and high vapour pressure, volatilization from soil would be rapid; half-lives of 0.2 and 0.5 days were reported for volatilization from soil at 1 and 10 cm incorporation, respectively. (Jury et al. 1984)	
Adsorption/desorption	A Koc of 0.40 was reported in "standard soil". (Jury et al. 1984) Based on the reported water solubility, a Koc of 56 was estimated. (Lyman et al. 1982)	
Mobility	Based on the reported and estimated Koc values, vinyl chloride will be expected to be highly to very highly mobile in soil. (Swann et al. 1983)	
Photochemical degradation in air	Gas phase vinyl chloride is expected to degrade rapidly in air by reaction with photochemically produced hydroxyl radicals with an estimated half-life of 1.5 days. (Perry et al. 1977) Products of reaction in the atmosphere include chloroacetaldehyde, HCl, chloroethylene epoxide, formaldehyde, formyl chloride, formic acid and carbon monoxide. (Muller & Korte 1977) In the presence of nitrogen oxides the reactivity of vinyl chloride is higher with a half-life of 3–7 hours. (Howard 1990)	
Photochemical degradation in water	In water no photodegradation was observed in 90 hours; however, degradation is rapid in the presence of sensitizers, such as might be the case in humic waters, or free radicalsas might be found in PVC manufacturing effluent streams. (Callahan et al. 1979)	
Hydrolysis in water	Hydrolysis will not be a significant loss process. (Mabey et al. 1981)	
Anaerobic degradation in soil	Vinyl chloride was approx 50% (20%) and 100% (55%) degraded in 4 and 11 weeks, respectively, in the presence (absence) of sand by methanogenic microorganisms under anaerobic conditions in laboratory scale experiments. (Brauch et al. 1987)	
Other information about bioaccumulation	Based on the reported water solubility, a BCF of 7 was estimated (Lyman et al. 1982). Based on the estimated BCF, vinyl chloride will not be expected to significantly bioconcentrate in aquatic organisms (Ly et al. 1977).	
LD50 values to mammals in oral exposure, mg/kg	500	orl-rat (Lewis & Sweet 1984)
LCLo values to mammals in inhalation exposure, ppm	20	30 min, ihl-gpg (Lewis & Sweet 1984)

2045 • 2-Vinylpyridine

100-69-6

Sumformula of the chemical	C7H7N
EINECS-number	2028798
Water solubility, mg/l	29700 (MITI 1992)
Melting point, °C	< -10 (MITI 1992)
Boiling point, °C	79–82 79 mmHg (MITI 1992)
Log octanol/water coefficient, log Pow	1.54 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

2046 • 4-Vinylpyridine

100-43-6

Water solubility, mg/l	> 10000 (MITI 1992)
Boiling point, °C	68–72 19 mmHg (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Bioconcentration factor, fishes	58–96 8w, Cyprinus carpio, conc 0.02 mg/l 48–96 8w, Cyprinus carpio, conc 0.002 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).
LD50 values to birds in oral exposure, mg/kg	100 orl-Agelaius phoeniceus (Schafer et al. 1983)
LC50 values to fishes, mg/l	1.57 48hr, Oryzias latipes (MITI 1992)

2047 • Warfarin

81-81-2

Synonyms	4-Hydroxy-3-(3-oxo-1-phenylbutyl)-quemarin 4-Hydroxy-3-(3-oxo-1-phenylbutyl)-coumarin 3-(α-Acetonylbenzyl)4-hydroxycoumarin
Sumformula of the chemical	C19H16O4
Products containing the chemical	"42" Extra Jyväsyötti * warfarin 0.5 g/kg (PESREG)
Use	Active ingredient in rodenticides.
State and appearance	Powder, white to pale cream colour (PESREG).
Odour	Slight odour (PESREG).
Molecular weight	308.35
Vapour pressure, mmHg	0.0000008 < 0.0001 Pa, 25 °C (PESREG)

UVW

Melting point, °C	162–166 (PESREG)
Other physicochemical properties	Insoluble in water. (PESREG) Soluble in acetone > 1000 mg/100ml. (PESREG)
LD50 values to mammals in oral exposure, mg/kg	3 orl-rat 331 orl-mus 200 orl-dog (Lewis & Sweet 1984) 253–393 orl-rat male 40–76 orl-rat female 174–190 orl-gpg 200–300 orl-dog (Hagan & Radomski 1953)
LD50 values to mammals in non-oral exposure, mg/kg	1400 skn-rat (Lewis & Sweet 1984)
LC50 values to fishes, mg/l	12 96hr, Rasbora heteromorpha (Tooby et al. 1975)

2048 • Win 29148a

22683-22-3

Other information about mammals	LDfr = 22.2 mg/kg, subacute, Deer mouse; ALD = 0.35–0.36 mg/kg, act, orl, Deer mouse (Virtanen & Nuuja 1987).

2049 • Xanthone

90-47-1

Effects on arthropods	LC50, 1 d: Aedes aegypti, 0.150 mg/l; Aedes taeniorhynchus, 0.460 mg/l; Culex quinquefasciatus, 0.092 mg/l (Borovsky et al. 1987).

2050 • Xylene

1330-20-7

Synonyms	Dimethylbenzene
Use	Solvent in resins, lacquers, enamels and rubber cements, in aviation fuel, and in the manufacture of polyester, pharmaceuticals, dyes, insecticides, asphalt and naphtha.
Odour	Threshold odour concentration in water: 1–2 mg/l (Zoeteman et al. 1974). Quality: sweet Hedonic tone: neutral to pleasant Threshold odour concentration absolute: 0.08 ppm 50% recognition: 0.27 ppm 100% recognition: 0.27 ppm Odour index 100% recognition: 29 222 (Hellman & Small 1974).
Molecular weight	106.17
Water solubility, mg/l	200
Boiling point, °C	137
Volatilization	Relative volatility (nBuAc=1) = 0.6

Half-life in water, days	0.23 at 25 °C (Mackay & Leinonen 1975)
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).
Metabolism in mammals	Xylene is thought to be well absorbed by the gastrointestinal tract, and distributed to the lipid-rich tissues. Metabolism in the liver is rapid, but the pathways differ slightly, depending on the isomer (Fawell & Hunt 1988). In man, about 60% of inhaled xylene is retained by the lungs (Sedivec & Flek 1976, Astrand et al. 1978). Percutaneous absorption also occurs readily (Engström et al. 1977). Although there are no data on gastrointestinal absorption, xylene would be expected to be readily absorbed in view of its lipophilic nature. The distribution of xylene in the body is dependent on the fat content of individual tissues. The highest levels of xylene are found in lipid-rich tissues such as the adipose tissue, subcutaneous fat, adrenal glands, brain and liver (Fawell & Hunt 1988). The metabolic pathways differ for each xylene isomer. The meta- and para-isomers are 80–90% metabolized to the corresponding toluic acids and glycine conjugates (Williams 1959). Only 60% of ortho-xylene is transformed to ortho-toluic acid, and of this roughly half remains free, about half is conjugated with glucoronide, and only 0.3% is conjugated with glycine (Bray et al. 1949, Ogata et al. 1970). Aromatic ring oxidation to hydroxyxylenes (xylenols) has also been reported for each isomer, but this appears to be only a very minor route (Bakke & Scheline 1970). Methylbenzylmercapturic acids have also been identified as metabolites of xylenes, though only transformation of ortho-xylene in this manner appears to be of any quantitative significance (Van Doorn et al. 1980). Xylene is excreted in the urine as methylhippuric acids, free toluic acids, toluogluronic acids, dimethylphenols and methylbenzylmercapturic acids. A small amount of unchanged xylene can be exhaled from the lungs (Sedivec & Flek 1976).
LD50 values to mammals in oral exposure, mg/kg	5000 orl-rat 4300 mixed xylenes, orl-rat (Wolf et al. 1956)
LCLo values to mammals in inhalation exposure, ppm	6700 mixed xylenes, ihl-rat (Carpenter et al. 1975)
Effects on the physiology of mammals	The xylenes are of low acute toxicity in experimental animals. At high doses their principal effects are CNS depression and membrane irritation. The xylenes also appear to be of low chronic toxicity, though they have not been tested by the oral route (Fawell & Hunt 1988). Fabacher & Hodgson (1977) were unable to demonstrate enhanced hepatic microsomal O- or N-demethylase activity, or changes in the liver weight/body weight ratio of mice given daily intraperitoneal injections of 100 mg/kg of xylene for 3 days. In another study, increased serum ornithine-carbamyl transferase activity and higher levels of hepato-lipids were found in guinea-pigs following intraperitoneal injection of 1 g/kg xylene in corn oil (Divincenzo & Krasavage 1974). Combined administration of ethanol and xylene appears to result in additive effects on both the CNS and hepatic enzyme activities (Elovaara et al. 1980, Savolainen 1980, Riihimäki et al. 1982). No significant changes in blood parameters were found in rats and rabbits exposed by inhalation to 690 ppm of mixed xylenes, 8 hours/day, 6 days/week for 130 days. Exposure of rabbits to 1150 ppm for 55 days in the same study was found to result in lowered numbers of erythrocytes and leukocytes, and an increase in platelet numbers (Fabre & Truhaut 1954). No myelotoxic effects were observed in rabbits given 300 mg/kg/day of xylene by subcutaneous injection for 6 weeks or 700 mg/kg/day of xylene for 9 weeks (Speck and Moeschlin 1968).

Health effects	Acute exposure to very high doses of xylene can cause erythema, dehydration, defatting and blistering of the skin, irritation of mucous membranes, peripheral vasodilation, giddiness, fatigue, 'drunkenness', narcosis and unconsciousness (Fawell & Hunt 1988). The most common effects of acute exposure to lower levels of xylene are CNS-related. Gamberale et al. (1978) exposed healthy men to 1300 mg/m³ of xylene in inspired air for 70 minutes, 30 minutes of which was spent on a bicycle ergometer (100 W). The authors reported clear evidence of performance decrement in three out of a battery of behavioural test. Changes in dopamine and noradrenaline levels in selected areas of the brain have been found in rats exposed by inhalation to 2000 ppm of xylene, 6 hours/day for 3 days (Andersson et al. 1981).
Carcinogenicity	There appears to be no information on the carcinogenicity of xylenes other than two skin-painting studies of inadequate length (Fawell & Hunt 1988). Although no evidence for carcinogenicity was found in two 6 month skin painting experiments in mice (Kennaway 1924, Berenblum 1941), these studies were of insufficient duration, and therefore only very limited conclusions can be drawn. Long-term studies of mixed xylenes (60% meta, 14% para and 9 % ortho- and 17% ethylbenzene) given by gavage at doses of 250 or 500 mg/kg to rats and 500 or 1000 mg/kg to mice, indicated no evidence of carcinogenicity (US National Toxicology Program 1986).
Mutagenicity	The xylenes do not appear to be mutagenic in the Ames test, but there is only limited information available in higher test systems (Fawell & Hunt 1988). All three isomers of xylene have given negative results for mutagenicity in the Ames test with Salmonella typhimurium, both in the presence and absence of either rat liver or hamster liver S-9, and at doses ranging from 1.0–500 μg/plate (Bos et al. 1981, Haworth et al. 1983). Xylenes have been shown not to be mutagenic in the Salmonella / microsome assay, bacterial DNA repair, not cause chromosome aberrations or sister chromatid exchanges in mammalian cells in vitro. Equivocal results were obtained in Drosophila germ cells but they did not cause chromosome aberrations in rat bone marrow in vivo (Dean 1978, 1985). Dose levels of 0.0152–1.52 mg/ml of xylene were not found to increase chromosome aberrations or sister chromatid exchanges in human lymphocytes in vitro (Gerner-Smidt and Friedrich 1978). Although no experimental data were given, Bos et al. (1981) reported that ortho-, meta- and para-xylene had given negative results for unscheduled DNA synthesis in primary cultures of rat hepatocytes. Mohtashamipur et al. (1985) report that ortho-, meta- and para-xylenes did not induce micronuclei in the bone marrow polychromatic erythrocytes of mice.
Teratogenicity	There is some evidence that xylene is teratogenic in mice at very high dose levels (Fawell & Hunt 1988). Xylene has been found at higher concentrations in cord blood than in maternal blood (Dowty et al. 1976). Two studies in mice have reported teratogenic effects of xylene. Nawrot and Staples (1980) dosed CD-1 mice by gavage with 0.3, 0.75 or 1.0 ml/kg/day of pure ortho-, meta-, or para-xylene on days 6–15 of gestation. Increased incidences of cleft palate and foetal resorptions were found at the two higher dose levels with the ortho- and para-isomers. In the other study, Marks et al. (1982) dosed CD-1 mice by gavage with 0.52, 1.03, 2.06, 2.58, 3.10 or 4.13 g/kg/day of a commercial xylene mixture (60.2% m-xylene, 9.1% ortho-xylene, 13.6% p-xylene and 17% ethylbenzene) in cottonseed oil, on days 6–15 of gestation. A significant increase in the incidence of malformed foetuses was found at the 2.06, 2.58 and 3.10 g/kg dose levels. The major malformation was again cleft palate. Other studies have noted embryotoxic effects, but failed to observe teratogenic effects in pregnant CFY rats exposed by inhalation to xylene isomers at up to 700 ppm on days 7–14 of gestation (Hudak & Ungvary 1978, Ungvary et al. 1980).
Other information	The xylenes have been regularly identified in the atmosphere and in water, but no data appear to be available on levels in food (Fawell & Hunt 1988).

2051 • m-Xylene

108-38-3

Synonyms	1,3-Dimethylbenzene
Use	Intermediate.
State and appearance	Colourless liquid.
Molecular weight	106.18
Vapour pressure, mmHg	6 20 °C
Melting point, °C	-48– -53
Boiling point, °C	139
Log octanol/water coefficient, log Pow	3.2 (Anon. 1988) 3.15 (Schwarzenbach et al. 1983) 3.2 (Sangster 1989)
Log soil sorption coefficient, log Kom	2.26 observed (Sabljic 1987) 2.53 calculated (Sabljic 1987)
Henry's law constant, Pa x m³/mol	530 (Anon. 1988) 675 calc. (Yaws et al. 1991)
Mobility	Equilibrium distribution: *mass %* air 99.33 water 0.54 solid 0.13 (Anon. 1988).
Chemical oxygen demand, g 02/g	2.62 5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	2.53 5 days (Bridie et al. 1979)
Half-life in air, days	0.062 1.5hr, estimated, under photochemical smog conditions in England (Verschueren 1983).
Total degradation in water	Biodegradation: 100% after 192hr (13 °C), incubation in the groundwater (natural flora) – in the presence of the other components of high-octane gasoline (0.100 ml/l) (Verschueren 1983).
Other information about degradation	Degradation of m-xylene: (see table below) a) Battermann 1984 b) Jamison et al. 1978 c) Kappeler & Whurman 1978 d) Hutchins & Ward 1984 e) Zeyer et al. 1986 f) Kuhn et al. 1985 (Anon. 1987b).
Bioconcentration factor, fishes	23.6 Anguilla japonica (Verschueren 1983)
LD50 values to mammals in oral exposure, mg/kg	5000 orl-rat (Lewis & Sweet 1984)

ENVIRONMENT	*INIT.CONC. mg/l*	*REDOX-COND.*	*TEMP. °C*	*DEGRADATION %/day*	*REF.*
water	0.312	aerobic	–	61/17	a
groundwater	0.0032	aerobic	13	100/8	b
groundwater	10	aerobic	10	100/7	c
soil	0.000062	aerobic	20	0/14	d
soil (adapted)	appr. 40	nitrate reducing	30	80/8	e
soil	0.0002	aerobic	20	100/1	f
soil	0.5	nitrate reducing	20	100/20	f

XYZ

LD50 values to mammals in non-oral exposure, mg/kg	14100	skn-rbt (Lewis & Sweet 1984)
LCLo values to mammals in inhalation exposure, ppm	2010	24hr, ihl-mus (Lewis & Sweet 1984)
TCLo values to mammals in inhalation exposure, mg/kg	424	6hr/6d, ihl-man (Lewis & Sweet 1984)
Maximum longterm immission concentration in air for plants, mg/m³	20	VDI 2306
Maximum longterm immission concentration in air for plants, ppm	5	VDI 2306
LC50 values to fishes, mg/l	38 9.2 16	14 d, Poecilia reticulata 96hr, Micropterus salmoides (Könemann 1979) 24hr, Carassius auratus (Anon. 1975)

2052 • o-Xylene

95-47-6

Synonyms	1,2-Dimethylbenzene Xylol o-Dimethylbenzene Methyltoluene 1,2-Xylene 3,4-Xylene	
Sumformula of the chemical	C8H10	
Use	Manufacture of phthalic anhydride; vitamin and pharmaceutical syntheses; dyes; insecticides; motor fuels. Manufacturing terephalic acid for polyester, solvent recovery plants; specialty chemical manufacture; manufacturing of isophthalic acid, aviation gasoline, and protective coatings. As a solvent for alkyd resins, lacquers, enamels, and rubber cements. In dye manufacturing, and as an asphalt and naphtha constituent. As a solvent for sterilizing catgut; and in microscopy as a cleaning agent and with Canada balsam as an oil-immersent in microscopy. Intermediate (99.9%).	
State and appearance	Colourless liquid. Will float and form slick on the surface.	
Odour	Sweet. Odour threshold: lower 0.26 ppm; medium 2.21 ppm; upper 4.13 ppm (Sax 1986). Odour threshold, air: 0.08 ppm; 0.17 ppm; odour threshold, water: 1.8 ppm (Sax 1986).	
Molecular weight	106.18	
Specific gravity (water=1)	0.863–0.880	
Vapour density (air=1)	3.7	
Conversion factor, 1 ppm in air=	4.41	mg/m³
Conversion factor, 1 mg/m³ in air=	0.23	ppm
Vapour pressure, mmHg	6.6–6.688 9	25 °C 30 °C
Water solubility, mg/l	68–175	25 °C
Melting point, °C	-25– -28	

XYZ

Boiling point, °C	144–144.4
Log octanol/water coefficient, log Pow	3.13 (Chin et al. 1986) 3.13 (Anon. 1988) 3.12 (Sangster 1989)
Henry's law constant, Pa x m³/mol	320 (Anon. 1988) 423.9 calc. (Yaws et al. 1991)
Volatilization	Based on a mass transfer equation to estimate evaporation rates for assumed conditions of 25 °C, and 1 m depth of water, the evaporation half-life for o-xylene was calculated to be 38.8 months (Sax 1986). The concentration of o-xylene was measured in test aquaria being used to conduct static bioassays. An initial concentration of 1.3 µl/l measured 32%, 82%, and > 99% loss after 24, 48 and 96 hours, respectively. An initial concentration of 4.6 µl/l measured losses of 33%, 85%, and > 99% after the same intervals, respectively; 9.3 µl/l measured losses of 23%, 49%, 95% and > 99% after 24, 48, 72, and 96 hours. These losses were believed to be primarily due to volatilization although other variables included changes in aquaria biomass, bacterial degradation and sorption (Sax 1986). A mass transfer equation was developed consistent with the conceptual model employed by Liss and Slater, with the resulting estimated volatilization half-life at 25 °C and 1 m water depth of 5.61 hours (Sax 1986).
Mobility	Equilibrium distribution: *mass %* air 98.92 water 0.89 solid 0.19 (Anon. 1988) Soluble in alcohol and ether; soluble in acetone, benzene, carbon tetrachloride and petroleum ether (Sax 1986).
Chemical oxygen demand, g 02/g	2.91 5 days (Bridie et al. 1979)
Biochemical oxygen demand, g 02/g	1.64 5 days (Bridie et al. 1979)
Other information about degradation	Pseudomonas aeruginosa was cultured in a synthetic medium containing o-xylene as the sole carbon source, no growth was observed. O-xylene was oxidized to o-hydroxymethylbenzoic acid (Sax 1986). None of the microorganisms obtained from 364 soil samples were found to utilize o-xylene as a sole carbon source (Sax 1986). Degradation of o-xylene:

ENVIRONMENT	*INIT.CONC. mg/l*	*REDOX-COND.*	*TEMP. °C*	*DEGRADATION %/day*	*REF.*
water	0.510	aerobic	–	86/17	a
groundwater	0.0016	aerobic	13	100/8	b
groundwater	10	aerobic	10	100/12	c
soil	0.000042	aerobic	20	0/14	d
soil	0.04	aerobic	–	95/18	e
soil	0.257	methanogen	17	78/280	f
soil	0.257	methanogen	17	> 99/840	f
sterile soil	0.257	methanogen	17	0/280	f
sterile soil	0.257	methanogen	17	34/840	f
soil	0.5	nitrate reducing	20	100/37	g

a) Battermann 1984
b) Jamison et al. 1976
c) Kappeler & Whurman 1978
d) Hutchins & Ward 1984
e) Zehnder 1984
f) Wilson et al. 1986
g) Kuhn et al. 1985
(Anon. 1987b).

XYZ

Metabolism in mammals	The penetration of o-xylene through the abdominal skin of rats was low (Sax 1986). Adult male Wistar rats were administered ipr injections of o-xylene. A 75% decrease in hepatic glutathione resulted within 3hr after treatment, however, this level returned to normal after 24hr. The result revealed direct conjugation of o-xylene with GSH does not occur, and therefore, the chemical must be bio-activated by other cellular enzymes before it reacts with GSH. In another experiment, the rats were given ipr injections of 3 mmoles/kg in 0.5 arachis oil to determine the excretion of thioethers in the urine. Ten percent of the dose was excreted and identified as N-acetyl-S-(o-methylbenzyl)-L-cysteine. A dose 0.5 mmole/kg resulted in 21% excreted. For both dosages, the excretion was almost complete within 24hr after administration (Sax 1986). Rats and guinea pigs excreted phenol in the urine after a subcutaneous injection of 0.1 ml o-xylene (Sax 1986). The absorption, metabolism and excretion of o-xylene was studied in four healthy men, aged 28–50, who were exposed to vapours (0.2 or 0.4 mg/l) for 8hr. The pulmonary retention was found to be independent of the level and duration of exposure with a mean value of 62.4%. The total amount exhaled after exposure was calculated by determining the percent retained in the subjects, approximately 5.3% for o-xylene. Urinary metabolites included unchanged o-xylene, glycine-bound toluic acids, 2,3-xylenol and 3,4-xylenol. Hydroxytoluic acids; toluylglucoronic acids, and free toluic acids were not detected in the urine. Concentrations of unchanged o-xylene in the urine increased slightly following the first 2hr of exposure, and were not detected following termination of exposure. The total amount (of unchanged xylene) excreted was ascertained to be 0.005% of the amount retained during exposure. The levels of toluric acid reached a maximum at the end of the exposure and then decreased rapidly, although, trace amounts were still detected after 4–5 d. The total amount of toluric acid excreted was 97.1% of the o-xylene retained during exposure. Of this amount, 68.5% was excreted eithin 24hr. Total excretion of the xylenol metabolites occurred within 1–2 d, following exposure and was calculated to be 0.86% of the retained o-xylene dose (Sax 1986).
Other information about metabolism	Ortho-xylene (900 mg/kg) was given orally to rats and metabolized to phenol, showing up in the blood approximately 6hr later. When benzene (300 mg/kg) was given with o-xylene, the amount of phenol formed increased and was in the blood approximately 18hr and excreted in the urine approximately 36hr later. Blood hippuric acid levels also increased after administration of combination of benzene and another solvent (Sax 1986). O-xylene, 100 mg/kg dissolved in 1 ml propylene glycol, was administered by stomach tube to rats. Exretion in the urine within 48hr showed 0.1% of the dose converted to 3,4-dimethylphenol. Small amounts of 2,3-dimethylphenol were also excreted. 2-methylbenzyl alcohol was detected as another metabolite (Sax 1986). Inhaled o-xylene vapours are either exhaled unchanged or oxidized to o-tolyglucuronic acid. A minor metabolic pathway is hydroxylation to o-xylenol which is excreted either unchanged or after conjugation with sulfate and glucuronic acid (Sax 1986). Following an 8hr inhalation of approximately 0.2–0.4 mg/l, the pulmonary retention by humans was 63.6%. Approximately 95 % of the dose was metabolized, and another 5% was eliminated by the lungs during a 3d desaturation period. Urinary elimination was negligible (Sax 1986).
LD50 values to mammals in oral exposure, mg/kg	4000 orl-rat 4300 orl-rat 3600 orl-rat (Sax 1986)
LDLo values to mammals in oral exposure, mg/kg	5000 orl-rat (Sax 1986)

LCLo values to mammals in inhalation exposure, ppm	6125 6920	12hr, ihl-rat ihl-mus (Sax 1986) 12hr, ihl-rat ihl-mus (Sax 1986)
TCLo values to mammals in inhalation exposure, mg/kg	150 1500 3000	24hr, ihl-rat, 7-14d preg. 24hr, ihl-rat, 7-14d preg. 24hr, ihl-rat, 7-14d preg. (Sax 1986)
TCLo values to mammals in inhalation exposure, ppm	200	inh-hmn (Sax 1986)
Effects on the physiology of mammals	Noradrenaline-induced respiration was inhibited by 31% in isolated hamster brown fat cells exposed to 1 mM o-xylene in vitro. The cell consentration was approximately 1E5 cells/ml and the temperature 37 °C. Ehrlich-Ladschutz diploid ascites tumor cells were incubated for 5 hours in vitro at 37 °C with 50 or 100 ppm o-xylene. The ability of o-xylene to induce an increase in the frequency of irreversibly injured cells at these consentrations was comparable to controls (Sax 1986). A long-term inhalation study of ortho-xylene in several species failed to show significant changes in body weight or hematological parameters after continuous exposure to 78 ppm of xylene vapour for 90 days, or after 30 repeated exposures to 780 ppm of xylene (Jenkins et al. 1970).	
Health effects	Can be absorbed through skin at slightly hazardous chronic levels. Recognition odour 1.8 ppm in air. May be narcotic at high concentrations (Sax 1986).	
Mutagenicity	Gene mutation – negative references (Sax 1986).	
Teratogenicity	Mammals negative references (Sax 1986).	
Effects on invertebrates	Southern armyworm (Prodenia eridania) in groups of 12 worms (5 th or 6 th instar) were fed 0.0135 mmole/g diet ad libitum for 3 days. Worms were sacrificed and analyzed for the effects on the microsomal oxidase activities in the gut tissue. The epoxidase (222%), N-demethylase (201%), NADPH-sytochrome c reductase (128%) and cytochrome P-450 (169%) enzyme activities were all greatly increased as compared to controls (100%) (Sax 1986).	
Effects on plants	The rate at which electrolytes were lost from sunflower leaves (Helianthus annus) after treatment with o-xylene was proportional to the phytotoxicity. Plants 3–5 weeks old were administered 2 ml o-xylene by pipette onto the abaxial surfaces of 5 g of the plant leaves. Leaves were the immersed in 100 ml deionized water. The leakage of salts was measured by electrodes and the changes in conductance. The rate of electrolyte loss was 255E4 per min; the value for the untreated controls was 16E4 per min (Sax 1986).	
Maximum longterm immission concentration in air for plants, mg/m³	20	VDI 2306
Maximum longterm immission concentration in air for plants, ppm	5	VDI 2306
Effects on wastewater treatment	0.1% seriously retarded sewage digestion (Sax 1986).	
EC50 values to microorganism, mg/l	9.2	15 min Microtox (Hermens et al. 1985)
LC50 values to crustaceans, mg/l	5.3 1.3 10–100	24hr, Crago franciscorum 96hr, Crago franciscorum 24hr, Daphnia magna (Sax 1986)

EC50 values to crustaceans, mg/l	3.82	2d, mbt, Daphnia magna (Holcombe et al. 1987)
LC50 values to fishes, mg/l	13	24hr, Carassius auratus (Anon. 1975)
	13.5	96hr, Salmo gairdneri (Walsh et al. 1977)
	16.1	4d, Carassius auratus
	16.1	4d, Lepomis macrochirus
	16.1	4d, Pimephales promelas
	16.1	4d, Catostomus commersoni
	8.05	4d, Salmo gairdneri (Holcombe et al. 1978)
	21	96hr, Pimephales promelas
	39	96hr, Poecilia reticulata
	13	24hr, Carassius auratus
	11	24hr, 96hr, Morone saxatilis (Sax 1986)
Other information about water organisms	Aplexa hypnorum; LC50, > 22.4 mg/l, 4d (Holcombe et al. 1987).	
Other effects on aquatic ecosystems	The algal Chorella vulgaris had a 50% reduction of cell numbers vs. controls after 1 day incubation at 20 °C with exposure to 55 ppm o-xylene. A log period of 1 day between inoculation and commencement of growth existed at concentration of 25 and 50 ppm, however, no recovery of growth was observed at 171 ppm. These cells differed morphologically: the chloroplast was bleached and was aggregated in the center of the cell, as were other cell contents (Sax 1986).	

2053 • p-Xylene

106-42-3

Synonyms	1,4-Dimethylbenzene	
Use	Intermediate.	
State and appearance	Colourless liquid.	
Molecular weight	106.18	
Vapour pressure, mmHg	6.5	20 °C
Water solubility, mg/l	198	25 °C
Melting point, °C	13	
Boiling point, °C	138.4	
Log octanol/water coefficient, log Pow	3.18	(Anon. 1988)
	3.15	(Schwarzenbach & Westall 1981)
	3.15	(Sangster 1989)
Log soil sorption coefficient, log Kom	2.52	observed (Sabljic 1987)
	2.53	calculated (Sabljic 1987)
Henry's law constant, Pa x m³/mol	440	(Anon. 1988)
	614.4	calc. (Yaws et al. 1991)
Mobility	Equilibrium distribution:	
		mass %
	air	99.18
	water	0.67
	solid	0.15
		(Anon. 1988).
Chemical oxygen demand, g O2/g	2.56	5 days (Bridie et al. 1979)

Biochemical oxygen demand, g 02/g	1.4	5 days (Bridie et al. 1979)
Half-life in air, days	0.1	2.4hr, estimated, under photochemical smog conditions in England (Verschueren 1983)
Total degradation in water	Biodegradation: 100% after 192hr (13 °C) – incubation in the groundwater (natural flora) – in presence of the other components of high-octane gasoline (0.100 ml/l) (Verschueren 1983).	

Other information about degradation

Degradation of p-xylene:

ENVIRONMENT	*INIT.CONC. mg/l*	*REDOX-COND.*	*TEMP. °C*	*DEGRADATION %/day*	*REF.*
water	0.312	aerobic	–	61/17	a
groundwater	0.001	aerobic	13	100/8	b
groundwater	10	aerobic	10	100/14	c
soil	0.000062	aerobic	20	0/14	d
soil	0.00025	aerobic	–	100/1	e
soil	0.04	aerobic	–	100/5	e
soil	0.5	nitrate reducing	20	100/20	f

a) Batterman 1984
b) Jamison et al. 1976
c) Kappeler & Whurman 1978
d) Hutchins & Ward 1984
e) Zehnder 1984
f) Kuhn et al. 1985
(Anon. 1987b).

LD50 values to mammals in oral exposure, mg/kg	5000	orl-rat (Lewis & Sweet 1984)
LC50 values to mammals in inhalation exposure, ppm	4550	4hr, ihl-rat (Lewis & Sweet 1984)
LCLo values to mammals in inhalation exposure, ppm	3460	ihl-mus (Lewis & Sweet 1984)
		ihl-rat (Harper et al. 1974)
		ihl-mus (Lewis & Sweet 1984)
		ihl-rat (Harper et al. 1974)
	4740	ihl-mus (Lewis & Sweet 1984)
		ihl-rat (Harper et al. 1974)
Teratogenicity	There were no indications of behavioural effects in the offspring of female rats exposed on days 7–16 of gestation to 3500 or 7000 mg/m³ para-xylene by inhalation (Rosen et al. 1986).	
Maximum longterm immission concentration in air for plants, mg/m³	20	VDI 2306
Maximum longterm immission concentration in air for plants, ppm	5	VDI 2306
LC50 values to fishes, mg/l	35	7d, Poecilia reticulata
	2	24hr, Micropterus salmoides (Könemann 1979)
	20.9	96hr, Lepomis macrochirus (Pickering & Henderson 1966)
	18	24hr, Carassius auratus (Bridie et al. 1979)

2054 • Xylenol

1300-71-6

Synonyms	Dimethylphenol
Sumformula of the chemical	C8H100
EINECS-number	2150893

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Total degradation in water	Biodegradation: 44.3% by BOD (on the upward trend) period: 14d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).
Ready biodegradability	Confirmed to be biodegradable (Anon. 1987).

2055 • 2,4-Xylenol

105-67-9

Synonyms	2,4-Dimethylphenol	
Sumformula of the chemical	C8H10O	
Use	Intermediate in manufacture of phenolic antioxidants; pharmaceutical manufacturing; plastics and resin manufacturing.	
State and appearance	Colourless needles.	
Molecular weight	122.18	
Melting point, °C	26	
Boiling point, °C	211.5	
Log octanol/water coefficient, log Pow	2.35	(Sangster 1989)
LD50 values to mammals in oral exposure, mg/kg	3200 809	orl-rat orl-mus (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	1040	skn-rat (Lewis & Sweet 1984)
LC50 values to crustaceans, mg/l	2.1	48hr, Daphnia magna (LeBlanc 1980)
LC50 values to fishes, mg/l	7.8	96hr, Lepomis macrochirus (Buccafusco et al. 1981)
	9.5	48hr, Pimephales promelas (Phipps et al. 1981)
	30 13	24hr, Cyprinus carpio 96hr, Tinca tinca (Meinck et al. 1970)
LOEC values to fishes, mg/l	3.11	grw, schr, Pimephales promelas (Holcombe et al. 1982)
NOEC values to fishes, mg/l	1.97	grw, schr, Pimephales promelas (Holcombe et al. 1982)
Other information about water organisms	Tetrahymena pyriformis; EC50, grw, 2 d, 130.51 mg/l (Schultz 1987)	

2056 • 2,5-Xylenol

95-87-4

Synonyms	2,5-Dimethylphenol	
Sumformula of the chemical	C8H10O	
Log octanol/water coefficient, log Pow	2.34	(Sangster 1989)
LC50 values to fishes, mg/l	3.2–5.6	96hr, Salmo gairdneri (Webb et al. 1976)
	10.8	Tilapia mossambica (Devi & Sastry 1987)

2057 • 2,6-Xylenol

576-26-1

Synonyms	2,6-Dimethylphenol	
Sumformula of the chemical	C8H10O	
Log octanol/water coefficient, log Pow	2.36	
LC50 values to fishes, mg/l	6.7	48hr, Pimephales promelas (Phipps et al. 1981)

2058 • 3,4-Xylenol

95-65-8

Synonyms	3,4-Dimethylphenol	
Sumformula of the chemical	C8H10O	
Log octanol/water coefficient, log Pow	2.23	(Sangster 1989)
LC50 values to fishes, mg/l	21 16 7	24hr, Cyprinus carpio 24hr, Rutilus rutilus 24hr, egg, Salmo trutta (Dore et al. 1975)

2059 • 3,5-Xylenol

108-68-9

Synonyms	3,5-Dimethylphenol	
Sumformula of the chemical	C8H10O	
Purity, %	100	
Use	Phenolic resins; coal for disinfectants.	
State and appearance	Colourless.	
Odour	Lower odour threshold: 1 ppm (Sax 1986).	
Molecular weight	122.13	
Specific gravity (water=1)	1.04	
Vapour pressure, mmHg	1	50 °C
Melting point, °C	64	
Boiling point, °C	219.5	
Log octanol/water coefficient, log Pow	2.37	(Sangster 1989)
Other physicochemical properties	Flammability slight. Combustion requires preheating. Toxic combustion products. Extreme danger. Enter with great care. Highly reactive. Slightly soluble. Phenols are typically susceptible to oxidation in air. This is accelerated with alkaline conditions. Easily chlorinated to become compounds with lower taste and odour thresholds. Subject to biodegradation (Sax 1986).	
Chemical oxygen demand, g O2/g	2.66	5 days (Bridie et al. 1979)
Biochemical oxygen demand, g O2/g	0.1	5 days (Bridie et al. 1979)

XYZ

Other information about degradation	Biodegrades at moderate rate (Sax 1986).
Other information about metabolism	Absorbed material is partly excreted by kidneys and partly oxidized (Sax 1986).
LD50 values to mammals in oral exposure, mg/kg	608 orl-rat 477 orl-mus 1313 orl-rbt (Sax 1986)
TDLo values to mammals in non-oral exposure, mg/kg	4000 skn-mus, 20W-I, tumorigenic (Sax 1986)
Health effects	Strong skin irritant. Absorption through skin can result in death in 30 minutes; subacute doses can damage kidneys, liver, pancreas, spleen, and may result in edema of the lungs. Symptoms come quickly and may include headache, dizziness, muscular weakness, dimness of vision, ringing in the ears, irregular and rapid breathing, weak pulse, dyspnea. May be followed by loss of consciousness. Highly toxic by all routes. – Chronic irritant. Moderately toxic by all exposure routes. Chronic poisoning causes digestive disturbances, nervous disorders, and skin eruptions (Sax 1986). Skin and eye irritation data: eye, rbt, 0.726 mg, severe (Sax 1986).
LD50 values to birds in oral exposure, mg/kg	> 113 orl-Agelaius phoeniceus (Schafer et al. 1983)
Effects on wastewater treatment	Chlorination drops taste threshold even further (Sax 1986).
LC50 values to fishes, mg/l	53 24hr, Cyprinus carpio 52 24hr, Tinca tinca 50 24hr, egg, Salmo trutta (Anon. 1973a) 34 24hr, Carassius auratus 22 96hr, Carassius auratus (Bridie et al. 1979)
Other information about water organisms	Toxic effects: Rotatoria and ciliates: 77 mg/l; Chlorella pyrenoidosa: 49–81 mg/l; Crustacea: 46 mg/l; Molluscs: 108 mg/l; Mastigophora: 154 mg/l (Sax 1986). Threshold of toxicity: bream, bleak: 5.0 mg/l, 8 mg/l; 18 mg/l; 20 mg/l; carp: 10 mg/l, Scenedesmus: 40 mg/l, 96hr; Microregma: 70 mg/l, 96hr; Escherichia coli: > 100 mg/l (Sax 1986). Lower toxic limit: perch 11 mg/l (Sax 1986). Lethal limit: minnows: 20 mg/l, 0.1hr; perch: 26 mg/l, 0.16hr; 16 mg/l, 0.16hr; 12 mg/l, 0.16hr; eels: 20 mg/l, 0.5hr; roach: 70 mg/l (Sax 1986).

Other information	Taste imparting characteristics: 0.001 ppm (Sax 1986). Will reduce BOD (Sax 1986). 50 ppm had no effect on photosynthetic oxygenation of algae (Sax 1986). Air pollution: extreme danger (Sax 1986)

2060 • 3,5-Xylyl N-methylcarbamate 2655-14-3

Sumformula of the chemical	C10H13O2N	
Water solubility, mg/l	600	(MITI 1992)
Melting point, °C	99.5–100.5	(MITI 1992)
Log octanol/water coefficient, log Pow	2.24	(MITI 1992)
Total degradation in water	Biodegradation: 1% by BOD period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).	
Bioconcentration factor, fishes	0.8–2.5 < 1.9	6w, Cyprinus carpio, conc 0.5 mg/l 6w, Cyprinus carpio, conc 0.05 mg/l (MITI 1992)
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987).	
LC50 values to fishes, mg/l	67	48 hr, Oryzias latipes, (MITI 1992)

2061 • Zinc and zinc compounds 7440-66-6

Molecular weight	65.37	
TCLo values to mammals in inhalation exposure, mg/kg	124	50min, ihl-hmn (Lewis & Sweet 1984)
Effects on amphibia	LC50 (96hr), 2.10 ppm, tadpoles of Rana hexadactyla (Khangarot et al. 1985).	
Effects on plants	Horse-bean (Vicia faba) plants were grown in a nutrient solution containing 2 mg Zn/l → root growth was reduced (Blanatik & Bobak 1974). Soybean seeds (Glycine max) were planted in acid-washed sand. Beginning 5 days after seed germination the sand was saturated with metal solutions: Zn at 1 ppm caused reductions in stem and foliage dry weights (leaves and stems contained 0.0104 mg Zn/g (Vesper & Weidensaul 1978).	
LC50 values to algae, mg/l	10	96hr, Navicula, Rachlin et al.1983
EC50 values to algae, mg/l	7.1	rpd, 96hr, Chlorella saccharophila (Rachlin et al. 1982)
LOEC values to algae, mg/l	0.03	rpd, schr, Selenastrum capricornutum (Bartlett et al. 1973)
LC50 values to crustaceans, mg/l	0.16 0.1 0.28 1 2.24	21d, Daphnia magna 48hr, without food, Daphnia magna 48hr, with food, D.magna (Biesinger & Christensen 1972) 57hr, Gammarus pulex (Martin & Holdich 1986) 96hr, Gammarus lacustris (DeMarch 1988)
EC50 values to crustaceans, mg/l	0.1	rpd, 21d, Daphnia magna (Biesinger & Christensen 1972)

LOEC values to crustaceans, mg/l	0.07	rpd, 21d, Daphnia magna (Biesinger & Christensen 1972)
LC50 values to fishes, mg/l	0.8	96hr, Salmo gairdneri (Spry & Wood 1984)
	2.86–3.78	96hr, Lepomis macrochirus (Patrick et al. 1968)
	0.12	sfd, 96hr, Morone saxatilis
	0.43	hrd, 96hr, Morone saxatilis
	0.43	1%., 96hr, Morone saxatilis (Palawski et al. 1985)
	60.3	96hr, Channa punctatus (Saxena & Parashari 1983)
	0.35–1.6	21d, Salmo salar (Falmer et al. 1979)
LOEC values to fishes, mg/l	0.051	grw, chr, flag fish (Spehar 1976)
	0.078	srv, chr, Pimephales promelas
	1.37	srv, schr, Salvelinus fontinalis (McKim 1977)
	0.18	rpd, chr, Pimephales promelas (Brungs 1969)
	0.64	srv, grw, schr, Salmo gairdneri
	0.26	srv, grw, schr, Salmo gairdneri (Sinley et al. 1974)
	0.173	rpd, chr, Poecilia reticulata (Pierson 1981)
NOEC values to fishes, mg/l	0.026	grw, chr, flag fish (Spehar 1976)
	0.145	srv, chr, Pimephales promelas
	0.53	srv, schr, Salvelinus fontinalis (McKim 1977)
	0.03	rpd, chr, Pimephales promelas (Brungs 1969)
	0.33	srv, grw, schr, Salmo gairdneri
	0.14	srv, grw, schr, Salmo gairdneri (Sinley et al. 1974)
Effects on the physiology of water organisms	Tilapia zillii, 1–4 days, 22 mg/l, biochemical effect; Clarias lazera, 1–4 days, 32 mg/l, biochemical effect (Hilmy et al. 1987b).	
Other information about water organisms	LC50 (96hr), 10.5 mg/l, Lymnea acuminata (Khangarot et al. 1982).	
Other information	Toxicity decreases when the hardness of water increases (Berglind & Dave 1984).	

2062 • Zinc carbonate 3486-35-9

Synonyms	Carbonic acid, zinc salt
Sumformula of the chemical	CO3.Zn
Use	As pigment in manufacture of porcelains, pottery, rubber, astringent; tropical antiseptic; cosmetics; and lotions.
State and appearance	White crystalline powder. Will sink.
Molecular weight	125.39
Specific gravity (water=1)	4.42
Other physicochemical properties	Nonflammable. Will emit carbon dioxide and zinc oxide in fires. Evolves carbon dioxide at 300 °C. Practically insoluble in water, 10 ppm at 15 °C.

Other information about degradation	Persistent (Sax 1986).
Other information about bioaccumulation	Food chain contamination potential moderate. Zinc will accumulate in some organisms, but is not considered to be bioconcentrative (Sax 1986).
Health effects	When heated, evolves zinc oxide fumes which can cause a disease known as brass founders ague or brass chills. Ingestion of zinc salts leads to an emetic reaction (Sax 1986). Eye, skin, respiratory, and mucous membrane irritant (Sax 1986). Skin contamination may produce irritation, rash, and reddening. Contamination of mucous membranes produces reddening and irritation. Exposure of eye may produce pain, photophobia and corneal damage. Inhalation may produce coughing and choking (Sax 1986). Zinc salts are astringent, corrosive to the skin, irritating to the gastrointestinal tract, and may act as emetics, where the emetic concentration in water may be between 675 and 2280 ppm. After large doses have been ingested, fatal collapse may occur as a result of serious damage to the buccal and gastroenteric mucous membranes. The zinc ion is too poorly absorbed to induce acute systemic intoxication. – When in fires or highly heated, zinc oxides are emitted which may act as a skin irritant and when inhaled give symptoms af metal-fume fever (Sax 1986). Chronic hazard level: Generally, zinc compounds have no cumulative effects. The continued administration of zinc salts in small doses has no effect in man except those of disordered digestion and constipation (Sax 1986).
Effects on wastewater treatment	Little effect on water treatment process since a level af 10 mg/l is required for an effect (Sax 1986).
LC50 values to fishes, mg/l	63 as zinc, 96hr, Pimephales promelas (Sax 1986)
Other information about water organisms	Salmo gairdneri, 0.0793 mg/g, 280 d, change in length and/or weight (Satoh et al. 1987b).
Other information	Taste threshold, lower: 6 ppm; medium: 27.2 ppm (Sax 1986).

2063 • Zinc dimethyldithiocarbamate 137-30-4

Synonyms	Zinc-bis-N,N-dimethyldithiocarbamate Ziram Bis(dimethyldithiocarbamato)zinc Zinc bis(dimethylthiocarbamoyl)disulfide
Sumformula of the chemical	C6H12N2S4Zn
Use	Fungicide.
Molecular weight	305.81
LD50 values to mammals in oral exposure, mg/kg	1400 orl-rat 400 orl-rbt 480 orl-mus (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	23 ipr-rat 73 ipr-mus 18 ivn-mus (Lewis & Sweet 1984)
LDLo values to mammals in oral exposure, mg/kg	100 orl-gpg (Lewis & Sweet 1984)
LDLo values to mammals in non-oral exposure, mg/kg	5 ipr-rbt 20 ipr-gpg (Lewis & Sweet 1984)

XYZ

Carcinogenicity	NTP carcinogenesis bioassay completed: results positive, rat; results negative, mus (Lewis & Sweet 1984).	
LD50 values to birds in oral exposure, mg/kg	100 100 > 100	orl-bwd (Lewis & Sweet 1984) orl-Agelaius phoeniceus orl-Passer domesticus (Schafer et al. 1983)
EC50 values to microorganism, mg/l	0.15 100	15 min Microtox (Van Leeuwen et al. 1985) Nitrification (Van Leeuwen et al. 1985)
EC50 values to algae, mg/l	1.2	rpd,96hr, Chlorella pyrenoidosa (Leeuwen et al. 1985)
LC50 values to crustaceans, mg/l	0.14 0.45	48hr, Daphnia magna (Leeuwen et al. 1985) act, Daphnia pulex (Nishiuchi & Hashimoto 1967)
LC50 values to fishes, mg/l	0.075 0.75	48hr, Cyprinus carpio (Nishiuchi & Hashimoto 1967) 96hr, Poecilia reticulata (Leeuwen et al. 1985)

2064 • Zinc(II)chloride 7646-85-7

Synonyms	Zinc dichloride Zinc chloride	
Sumformula of the chemical	Cl2Zn	
Purity, %	95	
Use	Dyes; mercerize cotton 2269; rubber; embalming; galvanizing iron; fireproofing; soldering; deodourant 2842; disinfectant; preserving; RR ties; etching metals; manufacture parchment paper; manufacture artificial silk; glue; manufacture vulcanized fiber 2655; magnesia; cement; petroleum oil; refining; printing; textiles; carbonizing; woolen goods; prod crepe 2221; prod crimping fabric; preserving anatomical specimens; sizing fabrics; weighing fabrics; microscopy; dehydrating agent; antiseptic; astringent; veterinary.	
State and appearance	White crystal or deliquescent solution. Will dissolve.	
Molecular weight	136.27	
Specific gravity (water=1)	2.907	
Vapour pressure, mmHg	100	610 °C
Melting point, °C	290	
Boiling point, °C	732	
Other information about degradation	Zinc can persist indefinitely as cation (Sax 1986). Removal os zinc in a soil column is not less than 99.7% for 300 mg/l solution; high pH, organic chelate, and phosphate reduce mobility; Cu reduces adsorption by plants; exchangeable zinc concentration in soil > 10 ppm may be injurious to plants (Sax 1986).	
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987). Can accumulate in gill tissue and bone. Potential for accumulation positive. Concentration factor for Zn: marine plants, 1000 x; vertebrates, oysters, 1000000 x; fish, 2000 x; freshwater plants, 4000 x; invertebrates, 40000 x; and fish Radioactive zinc (Zn-65) has been found to concentrate on plants, milk, and aquatic life. Food chain contamination potential positive (Sax 1986).	
LD50 values to mammals in oral exposure, mg/kg	350 350 200	orl-rat orl-mus orl-gpg (Lewis & Sweet 1984)
LD50 values to mammals in non-oral exposure, mg/kg	31	ipr-mus (Lewis & Sweet 1984)

XYZ

LDLo values to mammals in non-oral exposure, mg/kg	30 173 11	ivn-rat ipr-gpg (Lewis & Sweet 1984) ivn-rbt (Sax 1986)
TDLo values to mammals in non-oral exposure, mg/kg	20 20.5 12.5 17	ipr-mus (Lewis & Sweet 1984) ipr-mus, 8d preg, teratogenic ipr-mus, 11d preg, teratogenic par-ham, tumorigenic (Sax 1986)
TCLo values to mammals in inhalation exposure, mg/kg	4800	30 min, ihl-man (Lewis & Sweet 1984)
Health effects	Direct contact can ulcerate skin, mumem (Sax 1986). Lime has not been shown chronic effects in man. A dose of 6 g has been reported as fatal to man. One of the more toxic zinc salts due to corrosive action. Emits toxic vapours when heated to decomposition (Sax 1986).	
Carcinogenicity	Believed by some to be carcinogenic (Sax 1986).	
Mutagenicity	Mutagen data: mma, sat, 90 mmol/l; cyt, hmn, lym, 0.3 mmol/l; cyt, rat, ast, 700 mg/kg; hma, mus, sat, 6 mg/kg; otr, ham, emb, 0.180 mg/l (Sax 1986).	
Other information about birds	TDLo, par, ckn, tumorigenic, 15 mg/kg (Sax 1986).	
Effects on wastewater treatment	Concentrations > 20 mg/l have a toxic effect on activated slugde (Sax 1986).	
EC50 values to crustaceans, mg/l	 14.5 1	* as zinc: 48hr, crab adult 48hr, crab larvae (Sax 1986)
LC50 values to fishes, mg/l	 136 7.2 0.43 1.2 0.41 0.64 0.67 0.96 4.76 3.3 4 0.11 0.24–0.56 0.41–0.83 0.56 1.1 0.1 0.1 3.2	* as zinc: 48hr, Branchydanio rerio, embryo 96hr, Salmo gairdneri, juvenile,hrd 96hr, Salmo gairdneri, juvenile, sft 96hr, Salmo gairdneri, juvenile,hrd 14d, Salmo gairdneri, juvenile, sft 14d, Salmo trutta, juvenile, sft 14d, Salmo clarci, juvenile, sft 14d, Salvelinus fontinalis, juv, sft 48hr, Salmo gairdneri,hrd 96hr, Lepomis macrochirus 48hr, Salmo gairdneri 96hr, steelhead trout, sft, 12 °C Salmo gairdneri, sft, 14 °C, 96hr Salmo gairdneri, sft, 6-10 °C, 96hr 96hr, Poecilia reticulata, sft, 24 °C 96hr, Oncorhynchus nerka, sft, 12 °C 48-96hr, Morone saxatilis, larvae 48-96hr, Morone saxatilis, fingerling 96hr, Phoxinus phoxinus (Sax 1986)
	0.17	24hr, Rasbora heteromorpha (Sax 1986)
	32	96hr, 10 °C, Zn, Alburnus alburnus (Linden et al. 1979)

XYZ

Effects on the physiology of water organisms	Salmo gairdneri, 1.25 mg/l, 4 d, change in enzyme activity (Castren & Oikari 1987). Salmo gairdneri, 0.0588 mg/g, 280 d, change in length and/or weight (Satoh et al. 1987b).
Other information about water organisms	Zinc increases susceptibility of salmon and other fishes to lethal ulceration caused by Aeromonas liquefaciens. Zn in 10 ppm range enhances viral-host action in rainbow trout cell line (Sax 1986). Odourless zinc poisoning causes inflamed gills in fish (Sax 1986). Daphnia magna, < 0.15 mg/l, Lake Erie, immobilized (Sax 1986). Biomphalaria glabrata, 33 days: 3.0 mg/l, lethal effect; 0.5 mg/l, reproductive effect (Muenzinger & Guarducci 1988). Ephydatia fluviatilis (Porifera; Spongillidae), 10 days, 0.0000001 M growth effect (Francis & Harrison 1988).
Other information	Air pollution: high (Sax 1986).

2065 • Zinc nitrate 7779-88-6

Synonyms	Nitric acid, zinc salt Zinc dinitrate
Sumformula of the chemical	N2O6Zn
Purity, %	100
Use	Mordant.
State and appearance	Colourless crystals. Will dissolve.
Odour	Odourless.
Molecular weight	189.39
Specific gravity (water=1)	2.07
Vapour pressure, mmHg	60 700 °C
Melting point, °C	36
Boiling point, °C	105 -6HOH
Other physicochemical properties	Solubility is dependent on pH, hardness, and alkalinity (Sax 1986).
Other information about degradation	Can persist indefinitely (Sax 1986).
Other information about bioaccumulation	Oysters and other sellfish concentrate ZN-65 by a factor of 100000. Concentration factor for Zn – marine plants = 1000 x. Invertebrates; a large part of this concentration occurs in the plankton on which they feed (100000 x). Fish 2000 x and freshwater plants 4000 x; invertebrates 40000 x and fish 1000 x. Half-life in total human body 933 days (Sax 1986). Radioactive Zn-65 has been found to concentrate in plants, milk, bone, mollusks, and aquatic life. Has been concentrated in pasture grass and passed on to grazing animals (Sax 1986).
Health effects	Zn has low toxicity to man, but nitrate can cause problems. – As far as can be determined the continued oral administration of zinc salts in small doses has no effects in man except those of disordered digestion and constipation. – Zn bearing water should not be used in acid drinks like lemonade because the resulting Zn compounds may be poisonous (Sax 1986).

Effects on plants	Small amounts of Zn are needed by most crops, but toxicity results when concentrations exceed a very low level. A Zn deficiency causes poor growth. – 2 mg/kg dry soil, peas, increased nitrogen content. – 1 mg/l, pines, required for normal growth. – 10 mg/l, oats, no injury. – 2 mg/l, cress, suppressed fungus disease. – 54–436 mg/l Zn, cress and mustard seeds in solution culture, delayed germination and greatly retarded growth (Sax 1986).
Effects on wastewater treatment	62.5 ppm inhibits sewage bacteria 50%. Concentrations > 20 mg/l were found to have a toxic effect on activated sludge (Sax 1986).
EC50 values to crustaceans, mg/l	* as zinc: 14.5 48hr, crab adult 1 48hr, crab larvae (Sax 1986)
LC50 values to fishes, mg/l	* as zinc: 7.2 96hr, Salmo gairdneri, juv,hrd 0.43 96hr, Salmo gairdneri, juv, sft 1.2 96hr, Salmo gairdneri, juv,hrd 0.41 14 d, Salmo gairdneri, juv, sft 4.76 48hr, Salmo gairdneri,hrd 4 48hr, Salmo gairdneri 0.24–0.56 96hr, Salmo gairdneri,sft, 14-15 °C 0.41–0.83 96hr, Salmo gairdneri, sft, 6-10 °C 0.64 14 d, Salmo trutta, juv, sft 0.67 14 d, Salmo clarci, juv, sft 0.96 14 d, Salvelinus fontinalis, juv, sft 136 48hr, Branchydanio rerio, embryo 19 72hr, Branchydanio rerio, embryo 3.3 96hr, Lepomis macrochirus (Sax 1986)
Effects on the physiology of water organisms	Salmo gairdneri, 0.050 mg/g, 280 d, change in length and/or weight (Satoh et al. 1987b).
Other information about water organisms	LC50, 6.67 mg/l as zinc, Tetrahymena pyriformis, 96hr; LC50, 32 mg/l as zinc, Ephemerella, 264hr; LC50, 16 mg/l as zinc, Acroneuria, 336hr (Sax 1986). 189 mg/l, 15hr, Daphnia magna, killed (Sax 1986).
Other information	Harsh metallic taste. – Zn poisoning causes inflamed gills in fish; no known adverse physiological effects except at very high concentrations. – Emetic concentration is 675–2280 mg/l. – Nausea and fainting sometimes result from 30 mg/l. – Has an unpleasant astringent taste (Sax 1986). Lower taste threshold: 5 ppm Zn; Upper taste threshold; 40 ppm Zn (Sax 1986). Air pollution: low (Sax 1986).

2066 • Zinc oxide

1314-13-2

Sumformula of the chemical	OZn	
Molecular weight	81.37	
LD50 values to mammals in oral exposure, mg/kg	7950	orl-mus (Sweet 1987)
LD50 values to mammals in non-oral exposure, mg/kg	240	ipr-rat (Sweet 1987)
TDLo values to mammals in oral exposure, mg/kg	6846	orl-rat, 1-22d preg. specific developmental abnormalities effects on newborn (Sweet 1987)

XYZ

TCLo values to mammals in inhalation exposure, mg/kg	600 ihl-hmn, lungs, thorax or respiration (Sweet 1987)
Other information about mammals	Skin and eye irritation data: skin, rabbit, 500 mg, 24hr, mild; eye, rabbit, 500 mg, 24hr, mild (Sweet 1987).
Mutagenicity	Mutation data: cyt, rat, ihl, 0.1 mg/m³; dnd, esc, 3000 ppm; dns, gpg, ihl, 5.3 mg/m³, 3hr, 6d (Sweet 1987).

2067 • Zinc phosphide

1314-84-7

Synonyms	Trizinc diphosphide
Sumformula of the chemical	P2Zn3
Purity, %	90–95%, commercially
Use	In rat and field mice poison preparations; medicine.
State and appearance	Dark gray crystals or powder. Will sink and slowly decompose.
Molecular weight	258.05
Specific gravity (water=1)	4.55
Melting point, °C	> 420
Boiling point, °C	1100
Other physicochemical properties	Nonflammable. May release flammable phosphine gas when wet. This gas is moderately explosive when exposed to flame. Irritating and toxic POx may be formed in fires. Insoluble in water, but will decompose slowly and release very toxic phosphine gas. Reacts slowly with water, more rapidly with dilute acid, to form phosphine gas, which is toxic and spontaneously flammable.
Other information about degradation	Persistent (Sax 1986).
Other information about bioaccumulation	Food chain contamination potential moderate. Zinc will accumulate in some organisms, but is not considered to be bioconcentrative (Sax 1986).
LD50 values to mammals in oral exposure, mg/kg	40 orl-mus 12 orl-rat (Sweet 1987) 40 orl-rat (Sax 1986)
LDLo values to mammals in oral exposure, mg/kg	250 orl-cat 40 orl-rbt 80 orl-wmn (Sweet 1987)
TDLo values to mammals in oral exposure, mg/kg	3600 orl-wmn (Sax 1986)
Other information about mammals	ALD = 42.0 mg/kg, act, orl, deer mouse (Virtanen & Nuuja 1987).

XYZ

Health effects	When heated, evolves zinc oxide fumes which can cause a disease known as brass founders ague or brass chills. Ingestion of zinc salts leads to an emetic reaction. Zinc phosphide affects the central nervous system (Sax 1986). Eye, skin, respiratory, and mumem irritant. May be absorbed through the skin in toxic amounts. Phosphine may be generated and is extremely toxic at low concentrations (Sax 1986). Skin contamination may produce burns that heal slowly with scar formation. Eye contamination may produce pain, photophobia, conjunctival edema, and corneal damage. At fire temperatures produces coughing, choking, and difficult breathing (Sax 1986). This material is very toxic to humans by ingestion; between 1 teaspoonful and 1 ounce may be fatal. Phosphine gas can also be released when this material is inhaled. It causes a depression of the central nervous system and irritation of the lungs, or there may be pulmonary edema, dilation of the heart, and hyperemia of the visceral organs. The acute oral LD50 for a rat is 40 mg/kg and the lowest lethal oral dose for a woman was 3600 mg/kg. – Chronic poisoning, characterized by anemia, bronchitis, and gastrointestinal, visual, speech, and motor disturbances are said to result from continued exposure to low concentrations (Sax 1986).
LD50 values to birds in oral exposure, mg/kg	23.7 orl-bdw (Sweet 1987) 23.7–237 orl-Agelaius phoeniceus 75.0–237 orl-Agelaius tricolor (Schafer et al. 1983)
Effects on wastewater treatment	Toxic; presents a fire hazard at treatment plant. The zinc reaction products will inhibit growth of sewage organisms at concentrations greater than 10 mg/l (Sax 1986).
LC50 values to fishes, mg/l	43 as Zn, 96hr (Sax 1986)
Other information	Taste threshold, lower: 6 ppm (Sax 1986).

2068 • Zinc sulfate

7733-02-0

Synonyms	Zinc vitriol Sulfuric acid, zinc salt Zincate
Sumformula of the chemical	ZnSO4
Products containing the chemical	Gosiavite
Purity, %	100
Use	Merchant dye, wood preservation, paper manufacture, chemical manufacture, rayon, preserving skins, medical.
State and appearance	Colourless crystals. Will dissolve in water.
Molecular weight	161.43
Specific gravity (water=1)	1.97
Vapour pressure, mmHg	60 700 °C
Water solubility, mg/l	965 25 °C
Melting point, °C	38
Degradation point, °C	600
Other information about degradation	Zinc can persist indefinitely as a cation (Sax 1986). High pH, organic chelates, and phosphate reduce mobility; copper reduces adsorption by plants (Sax 1986).

XYZ

Other information about metabolism	Radioactive zinc (Zn-65) has been found to concentrate in plants, milk, and aquatic life (Sax 1986).	
Other information about bioaccumulation	Confirmed to be non-accumulative or low accumulative (Anon. 1987). Can accumulate in gill tissues and bone. Potential for accumulation positive. Concentration factor for zinc: marine plants 1000 x, oysters 100000 x, fish 2000 x, freshwater plants 4000 x, invertebrates 40000 x, and fish 1000 x. Half-life in total human body is 933 days (Sax 1986).	
LD50 values to mammals in oral exposure, mg/kg	1891	orl-mus (Sax 1986)
LD50 values to mammals in non-oral exposure, mg/kg	258 29	ipr-rat ipr-mus (Sax 1986)
LDLo values to mammals in oral exposure, mg/kg	2200 2000	orl-rat orl-rbt (Sax 1986)
LDLo values to mammals in non-oral exposure, mg/kg	330 50 1.5 78 66 300 23	scu-rat ivn-rat scu-mus scu-dog ivn-dog scu-rbt ivn-rbt (Sax 1986)
TDLo values to mammals in oral exposure, mg/kg	333 193000 45 106	orl-rat, 1-18d preg, teratogenic orl-dom, 6-20d preg, teratogenic orl-hmn, 7D-C orl-hmn (Sax 1986)
TDLo values to mammals in non-oral exposure, mg/kg	2 3.625	ivn-ham, 8d preg, teratogenic scu-rbt,5D-C, tumorigenic (Sax 1986)
Health effects	Skin and eye irritation data: eye, rbt, 0.420 mg, moderate (Sax 1986).	
Mutagenicity	Mutagen data: sln, dmg, orl, 5 mmol/l; cyt, rat, ast, 1g/kg; otr-ham, emb 0.200 mmol/l (Sax 1986).	
Effects on wastewater treatment	1000 ppm severely inhibited sewage digestion; concentrations > 20 mg/l were found to have a toxic effect on activated sludge (Sax 1986).	
EC50 values to algae, mg/l	0.25	0.17d, pht, Scenedesmus quadricauda (Starodub et al. 1987)
LC50 values to crustaceans, mg/l	1.17 0.69 0.92 0.2 4.3	1d, Daphnia magna 2d, Daphnia magna (Khangarot et al. 1987) 2d, Daphnia magna (Hall et al. 1986) 4d, Macrobrachium carcinus (Correa 1987) 96hr, 21 °C, Zn, Nitocra spinipes (Linden et al. 1979)

EC50 values to crustaceans, mg/l	52.3 2d, mbt, Asellus aquaticus 18.2 4d, mbt, Asellus aquaticus 121 2d, mbt, Crangonyx pseudogracilis 19.8 4d, mbt, Crangonyx pseudogracilis (Martin & Holdich 1986) 1 1d, mbt, Daphnia magna 0.56 2d, mbt, Daphnia magna (Khangarot & Ray 1987) 14.5 as Zn, 48hr, crab adult 1 as Zn, 48hr, crab larvae 110 48hr, shrimp (Sax 1986)
LC50 values to fishes, mg/l	1.7 96hr, Poecilia reticulata (Pierson 1981) 33.3 96hr, Barbus conchonius (Pant et al.1980) 7.6 96hr, Pimephales promelas (Kemp et al. 1973) 13.0–33.0 4d, Tilapia zillii 26.0–52.0 4d, Clarias lazera (Hilmy et al. 1987) 20.96 4d, Pimephales promelas (Hall et al. 1986) > 1.0–24.0 2d, Salmo gairdneri (Shazili & Pascoe 1986) 2.4 4d, Salmo gairdneri 2.6 4d, Salmo gairdneri (Meisner & Hum 1987) 19 as Zn, 72hr, Branchydanio rerio, embryo 136 as Zn, Branchydanio rerio, embryo 6714 as Zn, 24hr, Branchydanio rerio, embryo 7.2 as Zn,96hr, Salmo gairdneri, juvenile,hrd 1.2 as Zn,96hr, Salmo gairdneri, juvenile,hrd 0.43 as Zn,96hr, Salmo gairdneri, juvenile, sft 0.41 as Zn,14d, Salmo gairdneri, juvenile, sft 0.64 as Zn,14d, Salmo trutta, juvenile, sft 67 as Zn,14d, Salmo clarci, juvenile, sf 0.96 as Zn,14d, Salvelinus fontinalis, juv., sft 4.76 as Zn, 48hr, Salmo gairdneri,hrd 1.5 as Zn, 96hr, Lepomis macrochirus 0.24–0.56 as zinc, Salmo gairneri, sft, 96hr 0.56 as Zn, 96hr, Poecilia reticulata, sft 1.1 as Zn, 96hr, Oncorhynchus nerka (Sax 1986) 0.14 as Zn, 96hr, Noemacheilus montanus (Joshi & Chamoli 1987) 3.6 6d, Pimephales promelas (Dawson et al. 1988) 10–15 mg/l, 3.75d, Salmo gairdneri (Woodall et al. 1988) 41.9 96hr, 10 °C, Zn, Alburnus alburnus (Linden et al. 1979)
EC50 values to fishes, mg/l	0.6 6d, Pimephales promelas (Dawson et al. 1988)
Effects on the physiology of water organisms	Salmo gairdneri, 0.0491 mg/l, 280 d, change in length and/or weight (Satoh et al. 1987b). Cyprinus carpio, 1 day, 2.3 mg/l, biochemical effect (Radi & Matkovics 1988). Macrobrachium carcinus, 0.25 days, 0.010 mg/l, oxygen consumption effect (Correa 1987).

Effects on the reproduction of water organisms	Branchydanio rerio, 0.710 mg/l, 16 d, change in percent hatch or time to hatch (Dave et al. 1987). Daphnia magna, 50 days, 0.025–0.100 mg/l, reproductive effect (Paulauskis & Winner 1988).
Other information about water organisms	LC50 (16d), 16 mg/l, Ephemerella (Kemp et al. 1973). LC50, Lymnaea luteola: 1 d, 7.0 mg/l – 21.8 mg/l; 4 d, 1.68–11.0 mg/l (Khangarot & Ray 1987). Zinc increases susceptibility of salmon and other fishes to lethal ulceration by Aeromonas liquefaciens. Zinc in 10 ppm range enhances viral-host in rainbow trout cell line (Sax 1986). Zinc poisoning causes inflamed gills in fish (Sax 1986). 16 mg/l, Acroneuria, 336hr, LC50 (Sax 1986). Algae, biomass effect: 2–10 days, 0.035–0.043 mg/l (Genter et al. 1987); 5–30 days, 0.540–48.4 mg/l (Genter et al. 1988). Population growth effect: Anabaena variabilis, 8 days, 100 mg/l, 8 days; Chlorella vulgaris, 4–16 days, 4–40 mg/l (Ahluwalia & Kaur 1988); Scenedesmus quadricauda, 15 days, 0.1–0.5 mg/l (Starodub et al. 1987b). Catla catla, 0.33–1.00 days, 20 mg/l, hematological effect (Rai 1987). LC50, Lymnaea luteola: 2 days, 3.8 mg/l; 4 days, 1.68 mg/l (Khangarot & Ray 1988). Protozoa, 2 days, 0.540–48.4 mg/l, population effect (Genter et al. 1988).
Other effects on aquatic ecosystems	Solubility is dependent on pH, hardness, and alkalinity (Sax 1986).
Other information	Degree of hazard to public health: Low toxicity. Irritant. Emits toxic vapours when heated to decomposition (Sax 1986). Air pollution: none (Sax 1986).

2069 • Zineb

12122-67-7

Use	Active ingredient in fungicides.	
LD50 values to birds in oral exposure, mg/kg	> 100 > 100	orl-Agelaius phoeniceus orl-Sturnus vulgaris (Schafer et al. 1983)
EC50 values to microorganism, mg/l	6.2 18	15 min Microtox (Van Leeuwen et al. 1985) Nitrification (Van Leeuwen et al. 1985)
EC50 values to algae, mg/l	1.8	96hr, rpd, Chlorella pyrenoidosa (Leeuwen et al. 1985)
LC50 values to crustaceans, mg/l	> 40 0.97	act, Daphnia pulex (Hashimoto & Nishiuchi 1981) 48hr, Daphnia magna (Van Leeuwen et al. 1985)
LC50 values to fishes, mg/l	250 > 40 > 40 7.2	96hr, Rasbora heteromorpha (Tooby et al. 1975) 48hr, Cyprinus carpio 48hr, Carassius auratus (Hashimoto & Nishiuchi 1981) 96hr, Poecilia reticulata (Van Leeuwen et al. 1985)

XYZ

2070 • Zink-O, O-dialkyl(C=4-5) dithiophosphate

Sumformula of the chemical	C16O4S4P2Zn; C20O4S4P2Zn
Melting point, °C	< -30 (MITI 1992)
Total degradation in water	Biodegradation: 0% by BOD (altered to O, O-dialkyl(C=4-5)dithiophosphate) period: 28d substance: 100 mg/l sludge: 30 mg/l (MITI 1992).

2071 • Zirconium compounds 7440-67-7

LC50 values to fishes, mg/l	1.08	28d, Salmo gairdneri (Birge et al. 1980)

2072 • Zytron 299-85-4

Synonyms	DMPA	
Other information about mammals	LDfr = 75.0 mg/kg/day, subacute, deer mouse (Virtanen & Nuuja 1987).	
LD50 values to birds in oral exposure, mg/kg	100 100	orl-Agelaius phoeniceus orl-Sturnus vulgaris (Schafer et al. 1983)

XYZ

Environment Guide

ENVIRONMENTAL PROTECTION

Environmental properties of chemicals • Volume 1

This handbook contains a comprehensive collection of data relating to the fate and behaviour of chemicals in the environment. The material is divided into two volumes. Volume 1 contains information on the physico-chemical properties, degradation, metabolism, bioaccumulation, toxicity and ecotoxicity of 2,073 chemicals. The most extensive part details the toxicity of chemicals to aquatic organisms. Volume 2 contains lists of abbreviations, a list of exposed species (Scientific–English–Finnish), and two indexes, one an alphabetical list of chemicals and the other a numerical list of these chemicals according to their CAS-numbers.

The handbook has been compiled from the Data Bank of Environmental Properties of Chemicals maintained by the Finnish Environment Institute. The information is derived from over 3,000 scientific publications, handbooks and other sources.

The contents of this publication are also available as a CD-ROM EnviChem 2.0, a PC database running under Windows operating systems.

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